Department of Chemistry

In academic year 2020, the Department of Chemistry had 30 full-time faculty (including one dual faculty appointment with the Institute for Medical Engineering and Science): five assistant professors, four associate professors without tenure, four associate professors with tenure, and 17 full professors. Six faculty members (Arup Chakraborty, Catherine Drennan, John Essigmann, Barbara Imperiali, Susan Solomon, and Steven Tannenbaum) have secondary appointments in Chemistry. Professor Alexander Klibanov transitioned to emeritus status. In addition to research in biological, inorganic, organic, materials and nanoscience, physical, and computational and theoretical chemistry, the department continued its strong programs in undergraduate and graduate education with 262 graduate students, 115 postdoctoral researchers, and 67 undergraduate chemistry majors (30 in Course 5 and 37 in Course 5-7).

Professor Mircea Dincă and Professor Jeremiah Johnson were promoted to full professor, Professor Yogesh Surendranath and Professor Adam Willard were awarded tenure, and Professor Gabriela Schlau-Cohen was promoted to associate professor without tenure (effective July 1, 2020). Also, Xiao Wang joined the faculty as an assistant professor of chemistry and a core member of the Broad Institute of MIT and Harvard.

Robert T. Haslam and Bradley Dewey Professor Troy Van Voorhis was named department head on October 1, 2019, replacing the interim department head, Camille Dreyfus Professor Stephen L. Buchwald.

Sadly, the Department of Chemistry saw the deaths of two emeritus professors due to complications from COVID-19 in spring 2020. Professor Daniel Kemp passed away on May 2 at the age of 83, and Professor Dietmar Seyferth died on June 6 at the age of 91.

In addition, Ramachandra Dasari, principal research scientist and associate director of the GR Harrison Spectroscopy Lab, which houses the MIT-Laser Biomedical Research Center, passed away peacefully of natural causes on April 12 at the age of 87.

Highlighted Faculty Awards and Honors

Arup Chakraborty was presented the Outstanding Graduate Faculty Award (based on student votes) for his classroom teaching in 2019. Also, he continues to serve as a member of the US Defense Science Board.

In June 2020, Catherine Drennan was honored with an MIT Committed to Caring Award in recognition of her attention and care in mentoring relationships with graduate students. The Committed to Caring program recognizes outstanding mentors and promotes thoughtful, engaged mentorship throughout the Institute.

Gabriela Schlau-Cohen, the Cabot Career Development Associate Professor, won a 2020 Camille Dreyfus Teacher-Scholar Award from the Camille and Henry Dreyfus Foundation. The award program supports the research and teaching careers of talented young faculty in the chemical sciences, and when choosing its teacher-scholars the foundation seeks those who demonstrate leadership in both research and education.

Alex K. Shalek, the Pfizer-Laubach Career Development Associate Professor of Chemistry, was named the recipient of the 2019–2020 Harold E. Edgerton Faculty Achievement Award. The award's selection committee recognized Shalek for "his leadership and pioneering spirit; his vision, inventiveness, and enthusiasm for mentorship and collaboration; and his tremendous contributions to a critical area at the intersection of science and medicine."

In May 2020 Susan Solomon, the Lee and Geraldine Martin Professor of Environmental Studies, was named the recipient of the Killian Award, MIT's highest faculty honor. Professor Solomon was recognized for her "leadership in working toward real-world solutions to address the global climate crisis."

In July 2019 Yogesh Surendranath, the Paul M. Cook Career Development Professor of Chemistry, was presented the Presidential Early Career Award for Scientists and Engineers by the White House.

Xiao Wang was named a 2020 Searle Scholar in recognition of her work in visualizing and understanding RNA modifications in brain function through in situ sequencing. The Searle Scholars Program supports high-risk, high-reward research across a broad range of scientific disciplines.

Graduate Student Support

In order to remain competitive with its peers, the Department of Chemistry at MIT continues to make graduate student support its highest fundraising priority with the objective of providing one full year of private support to every admitted graduate student (of whom there are approximately 50) during the five years it takes to complete the PhD requirements. Members of the Chemistry faculty are grateful to the following individuals for their continued support toward meeting this critical and ambitious goal:

Ping S. Chu PhD '80

Michael E. Strem

Merece Johnson

Daniel C. Harris SB '68 (V) and Sally L. Harris

Kin Chun T. Luk PhD '77 and Yuen-Kwan Luk

Jeffrey I. Steinfeld SB '62

T-Y and Amy L. Shen

Gregory C. Fu SB '85

Stephen L. Buchwald and Susan G. Haber

Jan Krouwer PhD '73 and Ruby Krouwer

Charles Wade PhD '65 and Kim Wade

Anonymous donor (Dietmar Seyferth Fund)

Kenneth M. Gordon family

A number of multi-donor endowed funds also provided support for graduate students at varying levels:

- 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
- Alan Davison Fellowship Fund
- Robert J. Silbey Memorial Fund
- Walter L. Hughes Memorial Fellowship Fund (expendable)

40th Anniversary of the Roger and Georges Firmenich Professorship in Natural Product Chemistry

Liz McGrath, individual giving officer for the Department of Chemistry, represented the department on a Resource Development Stewardship/Communications team project to produce *The Freedom to Innovate*, a 25-page coffee table book celebrating the 40th anniversary of Roger and Georges Firmenich's establishment of the Firmenich Professorship in Natural Product Chemistry. Connections with the Firmenich family are credited largely to late chemistry professor George H. Büchi, whose role as a long-time Firmenich consultant forged the Institute's bond with the company. The book will be presented to Firmenich board member Antoine Firmenich SB '88 and family members who plan to pay a post-pandemic visit to the campus.

Roger Firmenich, George Büchi, and Georges Firmenich together at an event in 1979.

Oral History of the Department of Chemistry

Professors emeritus Frederick D. Greene and Dietmar Seyferth participated in an oral history video project filmed over a period of approximately 12 months and completed shortly before Professor Seyferth was admitted to a care facility following a fall. While in the care facility Professor Seyferth contracted COVID-19 and, sadly, passed away from the virus on June 6, 2020.

Arthur C. Cope Professor Rick Danheiser conducted the interviews for the video series, with questions spanning 1953, when Professor Greene first arrived at MIT, to Professor Seyferth's subsequent arrival in 1957. Liz McGrath coordinated the series and conducted archival research, and Emrick Elias, former senior administrative assistant to the department head, undertook the role of videographer. The series has been edited by MIT Video Productions. Images for use in the series have been sourced in the Department of Chemistry, received from alumni, and identified in the MIT Museum. Further archival materials will be secured when the MIT Archives reopen.

Professors Dietmar Seyferth and Fred Greene sit side by side as seen from the recording window of a video camera.

Fundraising for Student-Run Groups

The student-run Chemistry Alliance for Diversity and Inclusion (CADI) supports the success of underrepresented identities at MIT. The group's goal is to ensure a safe, inclusive, and supportive environment that encourages the success of all underrepresented communities. CADI is committed to enriching experiences within the Department of Chemistry and assisting individuals to fully realize their potential in both their academic and professional chemistry pursuits.

Fundraising for CADI kicked off in December 2018 with an anonymous gift of $5,000 and reached endowment level as of June 2020. The following alumni and friends generously provided matching gifts during MIT's 24-hour challenges when CADI was the department's featured fund: Timothy J. Cronin PhD '65, Lawrence K. Fish, Professor Stephen L. Buchwald, Susan G. Haber, Laurel Heckman PhD '18, Theresa C. Kavanaugh PhD '92, James F. Kronauge PhD '87, and Scott Rocklage PhD '82. Many individuals supported the challenges, and others made annual gifts. Industry support was provided by Johnson Matthey, the Dow Chemical Company, Pfizer Inc., and Bristol Myers Squibb.

Fundraising for another student-run group, Women in Chemistry (WIC), kicked off in October 2017 and reached endowment level in 2018. WIC endeavors to enrich the experiences of graduate student and postdoctoral women in the Department of Chemistry through professional development, mentorship, outreach, and community building.

The department is also actively seeking gifts to endow a third student-run group, the Chemistry Graduate Student Committee (CGSC), which fosters community through departmental social events, forums, and intramural sports teams; an annual career panel series in which alumni share insights on careers in industry, consulting, law, science policy, and academia; and other activities. CGSC advocates on behalf of graduate students in regular meetings with the department head, faculty, the chemistry department administration, and Institute representatives.

Alumni and Friends Reception

With the arrival of the COVID-19 pandemic and the subsequent shutdown, the annual alumni and friends reception hosted by the School of Science and Department of Chemistry, which had been scheduled for May 4, 2020, was postponed indefinitely. The chosen speakers for the evening, Professors Mei Hong and Daniel L. Suess, will again be invited to speak when the event is rescheduled at a post-pandemic time when it is safe to host the gathering.

Alumni and Friends of the Department of Chemistry Webinar

A webinar featuring chemistry professors working to combat COVID-19 took place on June 30, 2020. The event was moderated by department head Troy Van Voorhis, and 362 attendees were treated to presentations given by Professors Hong, Laura L. Kiessling, Bradley L. Pentelute, Alex K. Shalek, and Timothy M. Swager by way of five-minute lightning talks highlighting the work the professors have pivoted toward in combating the virus. After a general Q&A session, attendees were invited to break-out rooms to ask further questions of individual speakers.

Named Lectures

The department welcomed the following named speakers during the fall of 2019:

- Boehringer Ingelheim Lecture in Organic Chemistry: Franziska Schoenebeck, Rheinisch-Westfälische Technische Hochschule Aachen University
- Merck-Banyu Lecture in Organic Chemistry: Aiko Fukazawa, Kyoto University
- Merck-Pfister Lecture in Organic Chemistry: Cathleen Crudden, Queen’s University

The spring 2020 lectures were cancelled and/or postponed due to the COVID-19 pandemic.

Serving the Institute

The Department of Chemistry provides key educational services to the Institute. During AY2020, the department taught 1,079 MIT undergraduate students in the areas of biochemistry and inorganic, organic, and physical chemistry. The department was also the home for 69 Undergraduate Research Opportunities Program (UROP) students, providing important mentoring relationships for students from a number of departments, including chemistry, biology, physics, brain and cognitive science, 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 67 majors across three years (30 in Course 5 and 37 in Course 5-7). Starting in fall 2019, Course 5 majors were able to select the ChemFlex Option for their degree in chemistry. The ChemFlex Option is designed to provide an education based on science, both for those who intend to pursue chemistry as a career and for those who plan to go into an allied field, such as biotechnology or scientific consulting, in which a sound knowledge of chemistry is important. This training can be tailored to the student's interests by the judicious choice of elective focus subjects that contribute to the major. So far six students have graduated under the ChemFlex Option, and eight students are currently pursuing the option. Examples of our students' focus areas include chemistry with solid state physics/materials, neuroscience, and science education.

This year, 24 students received SB degrees in chemistry, 13 in Course 5 (four with the ChemFlex Option) and 11 in Course 5-7. In exit surveys, we found that 38% of the members of the Class of 2020 will be attending graduate school, 8% will be attending medical school, 25% will be working, and 13% have other immediate plans such as a gap year or military service. 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. All of the members of the Class of 2020 worked in a research group at least once during their degree program, conducting research alongside faculty, postdocs, and graduate students, and so far 85% of the members of the Class of 2021 and the Class of 2022 have worked in a group at least once.

Chemistry Teaching Assistants

Our graduate student teaching assistants (TAs) are some of the best at MIT. In fall 2019 and during the 2020 Independent Activities Period, students gave 73% of our TAs a 6.0 or higher rating on a 7.0 scale. Of the TAs in this percentile, 74% received a rating of 6.5 or higher.

Undergraduate Awards

Undergraduate awards were presented at the 2020 virtual commencement celebration on May 28.

- First-Year Chemistry Achievement Award (for outstanding academic achievement in chemistry): Jeffrey Shi
- Outstanding Sophomore Achievement Award (for outstanding achievement in academics, research, and service to the Department of Chemistry): Alex Li
- Outstanding UROP Presentation Award (for outstanding undergraduate research and in recognition of the best presentation at the 2019 Chemistry UROP Symposium): Agata Bikovsteva

- Alpha Chi Sigma Award (for outstanding achievement in scholarship, research, and service to the Department of Chemistry): Alexander Alabugin
- Research Award (for outstanding contributions in the area of research): Chun-Ting Liu, Miguel Aguilar Ramos, Yunyu Yang, and Sherry Zhou
- Royal Society of Chemistry Certificate of Excellence (for outstanding scholarship): Erin Grela, Madeleine Kline, Rebecca Sloan, Ruth Tweedy, Leon Yim, and Sherry Zhou
- Service Award (for significant contributions in the area of service to the Department of Chemistry): Gabriela Cazares and Darnell Granberry
- Phi Beta Kappa 2020 inductees: Erin Grela, Samuel Solomon, and Ruth Tweedy
- Teaching Assistant Awards: Rueven (Beny) Falkovich, JoLynn Giancola, Landon Kilgallon, Valerie Lensch, Soohyun Lim, Audrey Norris, Yana Petri, Sarah Quinn, Brighton Skeel, Stephanie Smelyansky, Kayla Storme, Carolyn Suh, Clair Travis, Axel Vera, Kathleen Wang, Sophia Weng, and Tiansi Xin
- Department of Chemistry Award for Outstanding Performance as a Graduate Grader: Elaine Reichert and Katherine Taylor

Doctoral and Master's Degree Recipients

Graduate Degree Recipients, September 2019

Name	Degree	Group
Samuel Bartko	PhD	Danheiser group
Julian Cooper	PhD	Radosevich group
Nicholas DeLateur	PhD	Weiss group
Allena Goren	PhD	Drennan group
Gyunghoon "Kenny" Kang	PhD	Drennan group
Richard Liu	PhD	Buchwald group
Jared Mattos	PhD	Radosevich group
Chloe Morgan	SM	Hong group
Christopher Richardson	PhD	Shoulders group
Nathan Ricke	PhD	Van Voorhis group
Mary Russell	PhD	Jamison group
Hyowon Seo	PhD	Jamison group
Ryan "Spencer" Shinabery	PhD	Buchwald group
Katherine Shulenberger	PhD	Bawendi group
Amanda Stubbs	PhD	Dincă group
Ashley Tong	PhD	Schlau-Cohen group

Graduate Degree Recipients, February 2020

Name	Degree	Group
Mohammad Murshid Alam	PhD	Kiessling group
Nadide "Hazal" Avci	SM	Movassaghi group
Timothy Barnum	PhD	Field group
Joseph Dennis	PhD	Buchwald group
Matthew Elkins	PhD	Hong group
Eric Hansen	PhD	Bawendi group
Cassie Jarvis	PhD	Kiessling group
Alexander Justen	PhD	Kiessling group
Trevor Nykaza	PhD	Radosevich group
Louis Papa	PhD	Shoulders group
Sanjay Prakadan	PhD	Shalek group
Jeffrey Rosenberg	SM	Surendranath group
Suan Tuang	PhD	Pentelute group
Frieda Zhang	PhD	Buchwald group

Graduate Degree Recipients, June 2020

Name	Degree	Group
Steven Cohen	PhD	Drennan group
Amro Dodin	PhD	Willard group
Ryan Duncan	PhD	Nelson group
Kaitlyn Dwelle	PhD	Willard group
Trevor Erickson	PhD	Field group
Michael Geeson	PhD	Cummins group
Alex Genshaft	PhD	Shalek group
Michael Gribble	PhD	Buckwald group
Samuel Kazer	PhD	Shalek group
Hyehwang Kim	SM	Cummins group
Soyoung Kim	PhD	Surendranath group
Nicole Moody	PhD	Bawendi group
Chase Olsson	PhD	Movassaghi group
Merjema Purak	PhD	Swager group
Phyo Pyae	PhD	Hong group
Marc Wadsworth	PhD	Shalek group
Lilia Xie	PhD	Dincă group
Jason Yoo	PhD	Bawendi group
Julia Zhao	PhD	Johnson group

As a result of the COVID-19 pandemic that forced the campus to vacate in March 2020, the graduates of 2020 were celebrated with virtual graduation celebrations held via Zoom on May 27 (for master's and PhD recipients) and May 28 (for undergraduate recipients). The events were livestreamed on YouTube for the graduates' families and friends to view and were presided over by department head Troy Van Voorhis and associate department head Sylvia Ceyer.

Faculty Research Highlights

Stephen L. Buchwald

The Buchwald research group focuses on the development of new synthetic methodology for the construction of carbon-carbon or carbon-heteroatom bonds based on fundamental mechanistic studies. In the past year, they have identified new reactivity of copper-hydride catalysis to enable highly selective olefin hydrofunctionalization for the synthesis of 1,3-disubstituted allenes, γ-amino alcohols, nitriles, pyrroles, indazoles, arenes with β-sterogenic centers, and homoallylic alcohols. The group's continuing projects with Professor Pentelute's group have resulted in techniques for the functionalization of complex biomolecules. Additionally, in collaboration with Chemical Engineering professor Klavs Jensen's group, they helped to develop a new way to optimize C-N cross-coupling reactions in flow and have created a platform for microfluidic electrochemistry.

Jianshu Cao

Microscopic objects such as electrons, excitation energies, and even chemical bonds are not localized in space and thus cannot be measured or even counted precisely. These microscopic objects follow the laws of quantum mechanics, exhibiting many striking features including "quantum coherence" (i.e., delocalization in space and time). The Cao group studies quantum coherence in light-harvesting complexes, organic aggregates, and molecular junctions and predicts their transport properties as well as spectroscopic signatures. Conceptually, the quantum nature of these chemical systems not only enhances their transport and optical features but also creates new quasi-particles by mixing with thermal environments or radiation fields, thus opening new avenues for chemical control.

Sylvia T. Ceyer

The Ceyer group continues to explore the remarkable growth at room temperature and below of a graphene overlayer that is catalyzed by the presence of Au on an Ni-Au surface alloy. The efficiency of the oxidation of covalent solid interfaces is probed using molecular beam surface scattering techniques to discern and mitigate the role of spin transitions in Si oxidation.

Arup K. Chakraborty

The Chakraborty lab continued its efforts to understand the mechanistic bases of how a systemic immune response to pathogens arises 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 continued to work on a project initiated in 2016 on understanding how genes critical for maintaining healthy cell states are regulated. Chakraborty has researched COVID-19 in 2020, and his HIV work has led to an immunogenic vaccine in monkeys. Chakraborty submitted a complete manuscript to The MIT Press for a general audience book focusing on viruses, pandemics, and immunity. He is also working on a book for physical scientists who want to enter, or have entered, the field of immunology.

Christopher C. Cummins

The Cummins lab reported the first catalytic reaction for the transfer of phosphinidenes to styrenic olefins, a useful process for synthesizing the three-membered ring compounds known as phosphiranes. In a collaborative study, the group investigated the selectivity of nitrosonium ion insertion into the bonds of tetrahedral AsP_3. In partnership with Professor Ronald Raines' lab, they showed that nucleoside tetraphosphates and pentaphosphates, prepared using Cummins' reagents and methodology, are potent inhibitors of the enzyme ribonuclease A. Addressing the question of the enzyme's stability, they isolated the first example of a phosphatetrahedrane, a molecule exhibiting the smallest bond angles of any known trivalent phosphorus compound. In the area of phosphorus sustainability, they argued that the production of white phosphorus en route to value-added phosphorus chemicals should be made obsolete.

Mircea Dinca

The Dincă group discovered a catalyst that converts ethanol, a bioderived fuel that is nevertheless difficult to transport and store due to its corrosive nature, to butanol, a much more benign fuel that has a higher octane rating and thus is a ready substitute for gasoline. The group also continued their fundamental forays into electrically conductive porous materials and demonstrated that the pi-stacking sequence of organic flat molecules can be an effective conduit for charge transport.

Catherine L. Drennan

All life encodes its genetic material in the form of DNA, made up of the same four deoxynucleotide building blocks (A, G, C, and T). In all organisms, ribonucleotide reductase (RNR) is solely responsible for converting ribonucleotides to their deoxynucleotide counterparts. Although structures of individual subunits of RNR were determined previously, in 2020 the Drennan lab published the first structure showing how RNR subunits come together to afford catalytic activity.

Robert W. Field

The transition state is a central concept of chemistry. A reacting system passes through the transition state in approximately 10^{-14} seconds. Therefore, textbooks report that it is impossible for experiments to reveal the transition state structure. How can a central concept be unobservable? The Field group has developed spectroscopic methods that tighten the net of observability. Vibrational polyads are robust patterns of energy levels that "break" at a transition state. H/D substitution serves as an on-off switch for tunneling between isomers. The vibrational population distribution of photofragments encodes the structure of the transition state at which the fragments are born.

Mei Hong

In 2019–2020, the Hong group determined the atomic-resolution structures of the influenza B virus M2 protein. The solid-state nuclear magnetic resonance (NMR) structures of BM2 in its closed (high pH) and open (low pH) states in phospholipid bilayers revealed that BM2 activates at low pH through a scissor-like motion, which differs from the transporter-type motion of the related influenza AM2. These closed and open structures should facilitate drug design to inhibit influenza B infections, which have become more dominant in recent flu seasons.

In addition, the group investigated the structure and lipid interactions of the HIV viral fusion protein gp41. Using an ectodomain-truncated construct of the protein, they showed that the two hydrophobic termini of gp41 associate with each other in lipid membranes, suggesting that the protein forms a hemifusion-like intermediate. They also investigated cholesterol binding to the C-terminal portion of gp41 using ^{19}F NMR and molecular dynamics simulations. They found that the trimeric protein binds three cholesterol molecules in close proximity, and binding depends not on a putative cholesterol-binding sequence motif but on the helix-turn-helix fold of the protein. These data suggest that gp41 may be recruited to the boundary of cholesterol-rich and cholesterol-poor regions of the lipid bilayer to incur membrane curvature.

The group also investigated the hydration of the tau amyloid fibrils found in neurodegenerative diseases. Using water-edited NMR experiments, they found that most of the β-sheet core is poorly hydrated and thus is surrounded by the dynamic, fuzzy coat segments of the protein. But two serine residues, S285 and S316, in the β-sheet core show enhanced hydration, suggesting that there is a small water channel inside the β-hairpin formed by the second and third microtubule-binding domains of the protein. These results suggest potential sites for inhibitor binding to disassemble these amyloid fibrils to slow disease progression, in addition to offering fundamental insight into the three-dimensional fold of this dynamically heterogeneous protein.

Timothy F. Jamison

The Jamison group, in collaboration with Klavs Jensen, developed a fully integrated, reconfigurable, automated benchtop system for the design, development, and execution of molecular synthesis. This system includes a machine learning approach, developed in the course of the collaboration, that designs syntheses with a level of expertise and accuracy comparable to that of advanced undergraduates and beginning graduate students. This invention simplifies the labor-intensive chemical experimentation process, thereby enabling researchers to focus their efforts on the more creative aspects of synthetic chemistry.

Jeremiah A. Johnson

The Johnson group established a method for the installation of cleavable silyl ether bonds into the backbone of common classes of polymers, enabling their degradation with tunable rates over several orders of magnitude. Additionally, they demonstrated a material that could switch among three different functional states in response to light and oxygen. In one state, the material could catalyze chemical reactions, enabling temporal control over the formation of desirable products. Lastly, the group introduced a new class of solvents that are exceptionally stable toward oxidation in the harsh environment of the Li-air battery cathode. This work has the potential to enable a new generation of energy storage devices.

Mohammad Movassaghi

The Movassaghi lab continues to focus on the development of new strategies and technologies for complex molecule synthesis. They recently reported unified enantioselective total syntheses and anticancer evaluations of all known communesin alkaloids and related derivatives, including the first total synthesis of communesins C-E and G-I and stereochemical revision of communesin I. Additionally, they disclosed their design, synthesis, and chemical study of a set of functional epidithiodiketopiperazines and evaluation of their activity against five human cancer cell lines, identifying potently anticancer and versatile molecules for future studies. The group continues to gain inspiration from nature in designing their chemical syntheses of complex molecules with high efficiency and stereochemical control in complex settings.

Elizabeth M. Nolan

The Nolan lab continued to investigate the metal-sequestering innate immune function of calgranulin proteins, including human calprotectin and MRP126, the single calgranulin homologue in birds and reptiles. In one particular new initiative, the metal-chelating and antimicrobial activity of chicken MRP126 was examined. This study revealed that chicken MRP126 selectively sequesters Zn(II) and that the presence of Ca(II) ions increases its binding affinity for Zn(II). This work is significant because it indicates that Ca(II)-dependent Zn(II) sequestration was a role of the last common ancestor of calgranulin proteins, with mammalian calprotectin subsequently evolving a broader metal-withholding repertoire.

Bradley L. Pentelute

The Pentelute group designs fully automated fast-flow machines to accelerate the chemical manufacture of sequence-defined biopolymers. They have built the world's fastest and most efficient machine, one that can produce thousands of amide bonds an order of magnitude faster than commercially available instruments. The machine is inspired by ribosome, which can make proteins in minutes. While the Pentelute group's fast-flow technology is not as fast as ribosome, it can form one amide bond in seven seconds. This technology not only facilitates rapid polypeptide generation but has enabled the group to carry out entire D-scans of proteins to investigate folding and functions. This past year, the technology was used to achieve stepwise total chemical synthesis of protein chains nearing 200 amino acids in length that retained the structure and function of native variants obtained via recombinant expression. Automated flow technology may solve the manufacturing problem for on-demand personalized therapies such as cancer vaccines.

Alexander T. Radosevich

In advancing the chemistry of low-symmetry phosphorus-based compounds in bond activation and catalytic transformations, the Radosevich group reported an improved procedure for reductive C-N coupling of nitroarenes and arylboronic acids involving phosphine/phosphine oxide redox cycling at a small ring phosphacyclic compound.

The group also described the application of this method to heterocycle synthesis and reported the nonspectator reactivity of a nontrigonal phosphorous triamide ligand in complex with a transition metal.

Ronald T. Raines

Wounds damage collagen, which is the most abundant component of human skin. Some bacteria have evolved the ability to make collagen. In 2019–2020, the Raines lab found that bacterial collagen enables bacterial cells to bind to damaged collagen and colonize wounds. This discovery suggests new strategies for preventing bacterial infections, which are a major health concern.

Gabriela S. Schlau-Cohen

In AY2020, the Schlau-Cohen group directly observed a hypothesized but previously unresolved pathway for converting excess energy to heat in plants and found that this pathway is activated through the interaction of multiple proteins. The group experimentally demonstrated that interaction between molecules and their surrounding solution can enhance the efficiency of energy transport. They found that when sugars bind to bacterial receptor proteins, the packing and dynamics of the proteins change inside the bacterium, which could be the mechanism by which bacteria move toward food.

Alex K. Shalek

There is a pressing need to understand the pathogenesis of severe acute respiratory syndrome coronavirus clade 2 (SARS-CoV-2), which causes the disease COVID-19. ACE2 is the cellular entry receptor for SARS-CoV-2, but the cell subsets that express it (and thus are likely viral targets) in host tissues, and the factors that regulate its expression, had yet to be elucidated. This year the Shalek lab, in collaboration with several researchers around the world, leveraged human, non-human primate, and mouse single-cell RNA-sequencing data sets collected across healthy and diseased conditions to uncover putative cellular targets of SARS-CoV-2, including lung type II pneumocytes, ileal absorptive enterocytes, and nasal goblet secretory cells. Strikingly, they found that the gene encoding ACE2 is an interferon-stimulated gene in human upper airway epithelial cells, but not in mice, suggesting that the virus could exploit species-specific interferon-driven up-regulation of ACE2, a tissue-protective mediator during lung injury, to enhance infection. Overall, their study has key implications for disease modeling and pre-clinical therapeutic development and highlights the power of the global scientific community to rapidly tackle new challenges through open sharing of data and ideas. In parallel, through local, national, and international partnerships, the Shalek lab pursued deep, mechanistic inquiries to elucidate the cellular and molecular features that inform tissue-level function and dysfunction across the spectrum of health and disease as a means of aiding in the design of therapeutic and prophylactic interventions to improve human health.

Matthew D. Shoulders

The Shoulders lab illuminated molecular details of the underlying protein misfolding defects that cause the debilitating bone disease osteogenesis imperfecta. Among other advances, they identified a key domain in collagen that the cellular quality control network engages to prevent secretion of defective collagens. The lab also discovered a novel role for the master regulator of cytosolic proteostasis, heat shock factor I, as an anti-HIV restriction factor.

Daniel L.M. Suess

The Suess group continued its study of the chemistry of iron-sulfur clusters. Researchers showed that reactive iron sites can be generated by protecting clusters from unproductive side reactions. This methodology was applied to studying reversible iron-carbon bond homolysis as it pertains to the mechanism of radical generation in the radical S-adenosylmethionine superfamily of enzymes.

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 general strategy for endowing molecular energy catalysts with reactivity profiles hitherto observed only in metals. In addition, they have developed a method for using renewable electricity to generate aqueous hydrogen peroxide and developed methods for quantifying the local electric field and pH environment at electrode surfaces.

Timothy M. Swager

Over the past year, the Swager group had a number of noteworthy scientific/technological innovations in sensing and separation methods. New generations of carbon nanotube–based resistivity sensors for ethylene, a universal plant hormone, were developed that were able to detect signals at 50 ppb levels (concentrations of 50 molecules of ethylene out of a billion gas molecules). These levels were sufficient to measure emissions from flowers, which are among the most sensitive plants to ethylene emissions. In the area of food safety, a new optical method that can be read with a smartphone was developed that is capable of detecting live *Listeria* in food. This method makes use of complex colloids in water wherein blocking and emissive dyes are positioned in different phases. In a new area of research, the Swager group teamed with the group of Assistant Professor Zachary Smith (Chemical Engineering) to create new gas separation membranes. These membranes are setting records in both stability and gas separation performance and will an expanding effort in the research group in the coming years.

Troy Van Voorhis

In the past year, the Van Voorhis group's major research accomplishment has been the development of bootstrap embedding as a method for highly accurate quantum mechanical energy calculations of large molecular systems. At a basic level, one can build up the energy of a large molecule by combining results from smaller, overlapping fragments. The key requirement is that one must match the different fragments in the overlapping regions, which the group did using novel bootstrap conditions. The resulting method predicts energies to within 0.1% for systems with hundreds of atoms and will have applications to the accurate simulation of solar energy materials.

Xiao Wang

The Wang lab started in summer 2019 and has come into shape in the past year. Their research focuses on developing and applying state-of-the-art chemical and biological tools to understand molecular events underlying brain connectivity and function. To this end, they have assembled an interdisciplinary team of students and postdoctoral researchers with backgrounds in chemistry, neuroscience, and computation. Despite the pandemic, the Wang lab successfully built the synthetic, analytical, and imaging set-ups in the lab and conducted a few proof-of-concept experiments.

Adam Willard

In AY2020, the Willard group focused primarily on studying two topics: the nanoscale properties of electrochemical interfaces and the behavior of excited electrons in disordered organic molecular semiconductors. Their work on electrochemical interfaces yielded a new theory for modeling reactivity within the electric double layer and a tool for efficiently simulating active electrode interfaces. This simulation tool revealed that electrolyte design rules for optimizing battery performance are not useful with microscopic battery architectures. The group's work in excited electrons has been aimed at developing new methods to accurately describe molecular structures in coarse-grained models of electronic dynamics. They have extended their methods to show how precisely designed molecular circuits can be used for quantum information processing.

Bin Zhang

The Zhang group introduced a consistent force field that enables, for the first time, accurate structural modeling for both ordered and disordered proteins. They applied the force field to study the folding of chromatin and uncovered different reaction pathways for the formation of regular fibril structures. In addition, they introduced an efficient simulation algorithm to explore the combination of multiple remodeling enzymes and transcription on nucleosome positioning. The group's study led to the discovery of a novel mechanism, a tug-of-war between two types of remodeling enzymes, that reconciles the conflicting trends found in nucleosome density profiles from different species.

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