# Department of Chemistry

In academic year 2019, the Department of Chemistry had 30 full-time faculty members (including one who held a dual 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. One faculty member—Alexander M. Klibanov—has a secondary appointment in Biological Engineering. Six additional faculty members—Arup K. Chakraborty, Catherine L. Drennan, Barbara Imperiali, Susan Solomon, Steven Robert Tannenbaum, and John M. Essigmann—have secondary appointments in Chemistry. Professor Alexander Klibanov announced his retirement in the summer of 2019; Professor Richard Royce Schrock and Professor JoAnne Stubbe moved on to emeritus status.

The department's members conducted research in biological, inorganic, organic, materials and nanoscience, physical, and computational and theoretical chemistry. The department also continued its strong programs in undergraduate and graduate education, with 273 graduate students, 124 postdoctoral researchers, and 62 undergraduate Chemistry majors (28 in Course 5 Chemistry and 34 in Course 5-7 Chemistry and Biology).

Professor Matthew D. Shoulders was awarded tenure, and Professors Yogesh Surendranath and Adam P. Willard were promoted to associate professor without tenure, effective July 1, 2018. Daniel L. M. Suess and Alison Wendlandt joined the faculty as assistant professors.

Robert R. Taylor Professor of Chemistry Timothy F. Jamison was offered the position of associate provost; he accepted, and completed his term as department head on June 30, 2019. Camille Dreyfus Professor of Chemistry and Associate Department Head Stephen L. Buchwald stepped in as interim department head.

## Highlighted Faculty Awards and Honors

In September 2018, the American Chemical Society named Professor Buchwald as the recipient of the Roger Adams Award in Organic Chemistry, sponsored by Organic Reactions Inc. and Organic Syntheses Inc. Professor Buchwald was chosen for this award in recognition of "breakthroughs in catalysis and ligand design that have had a profound impact on the synthesis of medicines, novel materials, agricultural agents, and natural products."

In September 2018, Professor Buchwald was awarded the 2018 Tetrahedron Prize for Creativity in Organic Chemistry. He shared the prize with Professor John Hartwig of the University of California, Berkeley. The Tetrahedron Prize is awarded on an annual basis for creativity in organic chemistry or bioorganic and medicinal chemistry.

In December 2018, the Technical University of Munich and Clariant Specialty Chemicals presented Professor Buchwald with the 2018 Karl Wamsler Innovation Award, presented in recognition of excellence in the field of catalysis. The award is given annually to promote excellent performance in the field of catalysis, including biocatalysis and industrial biotechnology.

In January 2019, Professor Buchwald was named one of seven laureates (across five scientific categories) honored with Israel's 2019 Wolf Prize. He shared the award in chemistry with Professor John Hartwig of the University of California, Berkeley. The prize was given for the development of the Buchwald-Hartwig amination, a process used to improve the synthesis of large organic molecules.

In June 2019, it was announced that Professor Rick L. Danheiser—the A. C. Cope Professor of Chemistry—would succeed Professor Susan S. Silbey as Chair of the Faculty. The chair, associate chair, and secretary of the faculty are the three elected officers of the MIT Faculty; they are assisted by the faculty governance administrator.

In September 2018, Associate Professor Jeremiah A. Johnson received an Arthur C. Cope Scholar Award, sponsored by the Arthur C. Cope Fund.

In February 2019, Professor Laura L. Kiessling—the Novartis Professor of Chemistry—was awarded one of the Institute's most respected honors: the Professor Amar G. Bose Research Grant, which supports work that is unorthodox and potentially world-changing. Professor Elizabeth M. Nolan also received the Professor Amar G. Bose Research Grant.

In May 2019, Professor Kiessling was named a winner of the 2019 Centenary Prize. Awarded annually by the Royal Society of Chemistry, the Centenary Prize is given to outstanding chemists who are also exceptional communicators.

In August 2018, Professor Bradley L. Pentelute received the 2018 Eli Lilly Award in Biological Chemistry. Established in 1934, and administered by the Division of Biological Chemistry of the American Chemical Society, this award is given in recognition of research in biological chemistry that is of unusual merit, independence of thought, and originality.

In July 2018, Professor Matthew D. Shoulders—the Whitehead Career Development Professor—received an Ellison Foundation Research Scholar Award from the American Cancer Society to support his project, New Connections: Stress, Proteostasis, Sugars, and Cancer. The Ellison Foundation's pioneering support for cancer care and research includes capital support for cancer facilities. The award will supply funding of roughly $800,000 over the next four years.

In September 2018, Professor Yogesh Surendranath—the Paul M. Cook Career Development Professor of Chemistry—was named one of 12 exceptional early career investigators from Canada and four other countries to join the Canadian Institute for Advanced Research Azrieli Global Scholars program. The program funds and supports researchers who are within five years of their first academic position, helping them build research networks and develop essential skills needed to become leaders in global research.

In September 2018, Professor Timothy Manning Swager—the John D. MacArthur Professor of Chemistry—was named the recipient of the ACS Award in Polymer Chemistry, sponsored by ExxonMobil Chemical Company. Swager's award was given in recognition of "the design, synthesis, and study of polymers with innovative molecular designs to create materials with superior sensory, electronic, optoelectronic, and mechanical properties."

In June 2019, Professor JoAnne Stubbe—the Novartis Professor of Chemistry, Emeritus—received the 2020 Priestley Medal, the American Chemical Society's highest honor.

## Development

On Wednesday, April 17, 2019, the first Dietmar Seyferth Lecture in Organometallic Chemistry was delivered by Henry Dreyfus Professor Christopher C. Cummins to an overflowing Room 6-120 lecture hall. A former Seyferth group member, Robert L. Lambert, PhD '73, established the endowed Seyferth lecture series in honor of his adviser, whom he credits with an invaluable education in the chemical sciences that led to his successful and fulfilling career. Professor Emeritus Dietmar Seyferth and his wife Helena were among the attendees, as were several former Seyferth graduate students, Chemistry Department faculty, students, postdoctoral associates, and friends. Frederick G. Keyes Professor Emeritus and 2005 Nobel Prize winner Richard R. Schrock gave the opening remarks.

*Dietmar Seyferth sits in the front row of his inaugural named lecture. Photo: Liz McGrath, 2019.*

The title of Professor Cummins's lecture was "Phosphorus-Element Bond-Forming Reactions," which covered three research areas currently being undertaken in his laboratory.

## Graduate Student Support

The department is grateful to the following individuals for establishing endowed funds, which will support graduate students in the coming summer. In some cases, the support will extend to the fall of 2019 and spring of 2020.

- Ping S. Chu, PhD '80—C.P. Chu & Y. Lai Fund
- Ping S. Chu, PhD '80—George H. Büchi Fellowship Fund
- Dr. Michael E. Strem—Strem Family Fund

- Mrs. Merece Johnson—David A. Johnson (1952) Fund
- Daniel C. Harris, SB ’68, and his wife, Sally L. Harris—Daniel S. Kemp Fellowship Fund
- Kin Chun T. Luk, PhD ’77, and his wife, Yuen-Kwan Luk—George H. Büchi/Kin Chin T. Luk Family Fellowship Fund
- Jeffrey I. Steinfeld, SB ’62—Ann and Paul Steinfeld Memorial Fellowship Fund
- T-Y Shen and Amy L. Shen—Amy Lin Shen Summer Fellowship Fund
- Gregory C. Fu, SB ’85—Gregory Fu (1985) Fund in Honor of K. Barry Sharpless
- Professor Stephen L. Buchwald and Susan G. Haber—Buchwald-Haber Family Fund
- Jan Krouwer, PhD ’73, and his wife Ruby Krouwer—Jan S. (1973) and Ruby Krouwer Fund
- Charles Wade, PhD ’65, and his wife Kim Wade—Charles (1965) and Kim Wade Chemistry Fund (to support undergraduate and graduate student research)
- Kenneth M. Gordon ’76 Scholarship Fund

Co-mingled endowed funds that also provide support for graduate students at varying levels include:

- 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
- Robert J. Silbey Memorial Fund
- Walter L. Hughes (1937) Memorial Fund (expendable fund)

## Dedication of MIT.nano

The much-anticipated MIT.nano building was completed on schedule in June 2018 and dedicated in October 2018. Two spaces in the state-of-the-art building were named for major supporters of the Chemistry Department. Judith E. Selwyn, PhD ’71 (Chemistry), and her husband, Lee L. Selwyn, PhD ’69 (Sloan School of Management), made a gift of $500,000; The conference room adjacent to the new chemistry undergraduate laboraries in the MIT.nano building is named in their honor for their generous gift. The director’s office in the Chemistry undergraduate teaching laboratories was named for the Fred J. Brotherton Foundation, which made a gift of $100,000 facilitated by Dr. William P. Brotherton, SB’72 (Chemistry).

### Instrumentation Facility Revitalization

On Tuesday, October 16, 2018, major donors to the revitalization campaign for the Department of Chemistry Instrumentation Facility celebrated the campaign's success with Chemistry faculty and staff. Guests enjoyed a buffet, cocktails, and tours of the facility. Located in the subbasement of Building 18 in the heart of the MIT campus, the facility supports and maintains a core area with analytical instruments.

During the evening, Director Walt Massefski and members of his team gave tours of the updated facility. In their welcoming remarks, Department Head Timothy F. Jamison and Dean of Science Michael Sipser expressed their deep appreciation to the chief supporters present, and to those who were unable to travel to the event. Professor Jamison also acknowledged the many other donors who had supported the initiative and expressed his appreciation to faculty and staff present who had been instrumental to the campaign's success.

### Alumni and Friends Reception

Professors Laura Kiessling and Daniel L. M. Suess shared their efforts to address some of the greatest challenges currently faced by the chemical sciences at an Alumni and Friends reception hosted by the Department of Chemistry and the School of Science on May 2, 2019.


*Laura Kiessling (left) and Daniel Suess (right) presented at the annual Alumni and Friends Reception. Photo: Justin Knight, 2019*

#### *Laura Kiessling, Novartis Professor of Chemistry*

"Every cell has a carbohydrate coat, and we are interested in how we can recognize bacteria that live in us, or that infect us," Kiessling explained in her presentation. "We hear a lot about the microbiome—it controls our weight, influences our health and disease in a lot of different ways, but we don't yet have a molecular understanding. Thinking about that carbohydrate coat as an ID and the proteins that we make as the ID checkers, that's a chemical language that is not yet understood."

The Kiessling laboratory focuses on chemical biology to elucidate the biological roles of carbohydrates, with an emphasis on learning new mechanistic concepts. All cells on Earth have a carbohydrate coat called the glycocalyx; this coat is poised to mediate or modulate biological and medical events. Given the emerging evidence that this coat serves as a crucial conduit of information, the laboratory is focused on elucidating how carbohydrates are assembled, how they are recognized, and how they function.

"We're very interested in how the carbohydrate-binding proteins in us might regulate the microbiome, as well as their roles in innate immunity, immunity and preventing microbes from invading us," said Kiessling. Figuring out how microbes make their carbohydrates is of particular importance. "If we can prevent them from making a critical carbohydrate, well, that's a new antibiotic!"

### *Daniel L. M. Suess, Class of '48 Career Development Assistant Professor of Chemistry*

"Chemistry is central to addressing our most pressing challenges—securing food and fuel for future generations and improving global standards of living, all while mitigating the effects of climate change," stated Suess. "Each of these goals relies on the development of efficient catalysts for difficult chemical transformations, and although the scientific community has now begun to undertake this work in earnest, Nature has been developing such catalysts—metalloenzymes—for billions of years."

Suess discussed his group's studies of the mechanisms of metalloenzymes and efforts to elucidate the principles that underlie metalloenzymes' remarkable reactivity and to uncover their roles in shaping the chemical composition of the biosphere. He highlighted his laboratory's recent advances in understanding the chemical mechanisms of some of the most ubiquitous metalloenzymes: those that harbor iron-sulfur clusters in their active sites. Using synthetic models of these active sites, the laboratory has stabilized intermediates featuring highly reactive iron-carbon bonds—species that are difficult to study in the enzymes themselves. This work points to potential roles for such organometallic intermediates in a diverse array of processes from fuel and fertilizer production to health and disease.

## Named Lectures

The department welcomed the following named speakers during the fall of 2018 and spring of 2019:

- Boehringer Ingelheim Lecture in Organic Chemistry: Helma Wennemers (ETH Zurich) and Jonathan Reeves (Boehringer Ingelheim)
- Merck-Banyu Lecture in Organic Chemistry: Naoya Kumagai (Institute of Microbial Chemistry, Tokyo, Japan)
- Novartis Lecture in Organic Chemistry: Sir Shankar Balasubramanian (University of Cambridge) and Christian Gampe (Novartis)
- John S. Waugh Lecture in Physical Chemistry: Professor Adriaan Bax (National Institutes of Health)

- Sigma-Aldrich Lecture in Organic Chemistry: Brett P. Fors (Cornell University)
- A.D. Little Lecture in Physical Chemistry: James Skinner (University of Chicago)
- Bristol-Myers Squibb Lecture in Organic Chemistry: Mark S. Taylor (University of Toronto) and Nicholas Meanwell (Bristol-Myers Squibb)
- TY Shen Lectures in Chemical Biology: Jonathan Weissman (University of California, San Francisco)
- Lord Lecture: Naomi J. Halas (Rice University)
- Dietmar Seyferth Lecture in Organometallic Chemistry: Professor Christopher C. Cummins (MIT)
- Büchi Lectures in Organic Chemistry: Dale L. Boger (Scripps Research Institute)
- Davison Lecture in Inorganic Chemistry: Hansjörg Grützmacher (ETH Zurich)
- Pfizer-MIT Lecture in Organic Chemistry: Marisa C. Kozlowski (University of Pennsylvania)
- Merck-Pfister Lectures in Organic Chemistry: Marc Hillmyer (University of Minnesota)
- MIT-Merck Lecture in Organic Chemistry: Rubén Martín (Institute of Chemical Research of Catalonia) and Subharekha Raghavan (Merck & Co., Inc.)

## Serving the Institute

The Department of Chemistry provides key educational services to the Institute. During AY2019, the Department of Chemistry taught 1,114 MIT undergraduate students in the areas of biochemistry and inorganic, organic, and physical chemistry. The department was also the home for 70 Undergraduate Research Opportunities Program (UROP) students and it provided mentoring relationships for students from a number of departments, including Chemistry, Mathematics, Physics, Chemical Engineering, Biological Engineering, and Materials Science.

## Chemistry Majors

The department continues to attract a very talented group of undergraduates to Course 5 Chemistry and Course 5-7 Chemistry and Biology; it had a total of 62 majors across the three years, 28 in Course 5 and 34 in Course 5-7. Starting in fall 2019, students majoring in Course 5 were able to select the ChemFlex option for their degree. The ChemFlex option is designed to provide an education based on science 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 course can be tailored to the student's interests by the judicious choice of elective focus subjects. Two members of the Class of 2019 selected the ChemFlex option; five students are now pursuing the ChemFlex option. The department expects a number of students from the Class of 2022 to select the ChemFlex option. Examples of students' focus areas include energy, and mineralogy and petrology.

This year, 17 students received bachelor's degrees in Chemistry; nine were in Course 5 (two with the ChemFlex option) and eight in Course 5-7. Self-reported data suggested that 35% of the Class of 2019 will attend graduate school, 24% will attend medical school, and 29% will be working. Plans for life after MIT were unknown for 12% of students.

### Undergraduate Research Opportunities Program

The UROP continues to be the capstone experience for the department's undergraduates. Some 94% of the Class of 2019 worked in a research group at least once during their degree program. In the Class of 2020 and the Class of 2021, 89% have worked in a research group at least once. Chemistry Department undergraduates have the opportunity to conduct research alongside faculty members, postdoctoral associates, and graduate students.

### Chemistry Department Teaching Assistants

The department's graduate student teaching assistants (TAs) are some of the best at MIT. This year, students gave 82% of Chemistry TAs a score of 6.0 or higher (on a 7.0 scale). Almost 65% received a score of 6.5 or higher.

### Undergraduate Awards

- **First-Year Chemistry Achievement Award**, for outstanding academic achievement in chemistry: Alex Liu, Heya Lee, and Vaishnavi Phadnis
- **Outstanding Sophomore Achievement Award**, for outstanding achievement in academics, research, and service to the Department of Chemistry: Siam Muquit
- **ACS Analytical Chemistry Award**, for outstanding achievement by a junior in experimental chemistry: Alexander Alabugin
- **Outstanding Undergraduate Research Opportunities Program Presentation Award**, for outstanding undergraduate research and in recognition of the best presentation at the 2019 Chemistry UROP Symposium: Alexander Alabugin
- **Alpha Chi Sigma Award**, for outstanding achievement in scholarship, research, and service to the Department of Chemistry: Minwoo Bae and Corin Wagen
- **Research Award**, for outstanding contributions in the area of research: Elizabeth Brewer, Katherine Chew, and Catherine Williamson
- **Royal Society of Chemistry Certificate of Excellence**, for outstanding scholarship: Angela Cai, Katherine Chew, Grayson Rodriguez, andYue Zhang
- **Service Award**, for significant contributions in the area of service to the Department of Chemistry: Tabrez Alam, Angela Cai, Songela Chen, Christopher Hillenbrand, and Clare Keenan
- **American Chemical Society Organic Chemistry Award**, for excellence in organic chemistry: Corin Wagen

## Special Recognition

### *Phi Beta Kappa 2019 Inductees*

- Minwoo Bae
- Angela Cai
- Katherine Chew
- Yue Zhang

### *Teaching Assistant Awards*

- Alex Callahan
- An Chu
- Amanda Cowfer
- Charlotte Farquhar
- Roger Jin
- James “Levi” Knippel
- Jet Lem
- Victoria Marando
- Amanuella Mengiste
- Gino Occhialini
- Elaine Reichert
- Jacob Rodriguez
- Katherine Walker
- Jinyi Yang

### *Excerpts from Teaching Assistant Evaluations*

> Best TA I’ve had at MIT. Our recitations flew by because I felt I was learning so much, and each time I left much more comfortable with my understanding of the material.
>
> Incredible organization, passion and encouragement for her students. Gave confidence to students when struggling.
>
> He clearly demonstrated his knowledge of the subject and was able to explain complex concepts in a manner which I could understand. His ability to answer my questions and prompt me to think deeper about the chemical phenomena occurring helped me learn a lot.
>
> THANKS FOR BEING A FABULOUS TA. She is super nice and really good at explaining concepts. She is also super easy to talk to and really supports students who are struggling in the class. Her office hours are really nice as well. And, the review handouts she prepares have saved my life so many times. Best TA.

So helpful!! Really knew what areas we found difficult and helped us with those as well as laid everything out in a straightforward way and was always super approachable and responsive!

[He] was an absolute godsend—his recitations and office hours were incredibly helpful, especially toward the end of the course when the material got more difficult. His teaching style is upbeat and approachable and he obviously cares a lot about his students. Best TA of the semester!

Always made sure I understood the concepts behind what the procedures were, made sure I was following (because I have less lab experience than the other people in the class) and helped me gain confidence with the new lab skills.

[He] is great. He taught so many things, both relevant to the course and just lab technique wise. He was very relaxed, yet organized and prepared. He had the perfect balance of everything that's needed for a TA, especially the one that has to spend a lot of time in lab per week.

Super kind and helpful. Answered every question we had and was able to differentiate instruction for the wide variety of people we had in the class. Awesome practice problems and super knowledgeable.

Before anything else, [he] is such a caring TA. He cares about his students endlessly and is probably one of the biggest reasons that I did well in the class. Not only was he understanding of the fact that sometimes we don't get things instantly, but he was just amazing at explaining things, and I could really feel that he wanted us to do well. This drove me to work hard for this class.

[She] is literally the best. She was so understanding of what being an undergrad was like and was very accommodating, while still helping us learn and having clear cut expectations that she followed through on.

## Doctoral and Master's Degree Recipients

**Degree Recipients, September 18, 2018**

| Name | Degree | Group |
|---|---|---|
| Tess Branon | PhD | Ting |
| Yisu Han | PhD | Ting |
| Myungwoon Lee | PhD | Hong |
| Zeyu Lu | PhD | Pentelute |
| Anthony Rojas | PhD | Buchwald |
| Wesley Transue | PhD | Cummins |
| Tran Truong | PhD | Swager |
| Kathleen White | PhD | Swager |
| Madeline Wong | PhD | Shoulders |

## Degree Recipients, February 19, 2019

| Name | Degree | Group |
|---|---|---|
| Chet Berman | PhD | Shoulders |
| Lisa Cunden | PhD | Nolan |
| Megan Jackson | PhD | Surendranath |
| Maciej Korzynski | PhD | Dincă |
| Chee Kong Lee | PhD | Willard |
| Qiao Li | SM5 | Kiessling |
| Elise Miner | PhD | Dincă |
| Wen Jie Ong | PhD | Swager |
| Valerie Ressler | PhD | Raines |
| Ian Windsor | PhD | Raines |

## Degree Recipients, June 19, 2019

| Name | Degree | Group |
|---|---|---|
| Eric Alt | PhD | Willard |
| Sophie Bertram | PhD | Bawendi |
| Phillip Calabretta | PhD | Kiessling |
| Yang-Ting Chen | PhD | Drennan |
| Kelley Danahy | PhD | Jamison |
| Deborah Ehrlich | PhD | Johnson |
| Yuwei Gu | PhD | Johnson |
| Rose Hadley | PhD | Nolan |
| Yuan He | PhD | Swager |
| Jennifer Hu | PhD | Dedon |
| Saki Ichikawa | PhD | Buchwald |
| Bryan Ingoglia | PhD | Buchwald |
| Yivan Jiang | PhD | Johnson |
| Liam Kelly | PhD | Jamison |
| Kellie Kolb | PhD | Shalek |
| Xian Li | PhD | Nelson |
| Hung Nguyen | PhD | Johnson |
| Seokjoon Oh | PhD | Surendranath |
| Matthew Pompeo | PhD | Movassaghi |
| Helena Qi | PhD | Kulik |
| Adam Reith | PhD | Dincă |
| Joseph Roddy | SM5 | Suess |
| Vera Schroeder | PhD | Swager |
| Hyun Shin | PhD | Nelson |
| Tho Tran | PhD | Jamison |
| Hendrik Utzat | PhD | Bawendi |
| Constantin Voll | PhD | Swager |
| Wade Wang | PhD | Hammond |
| Jessica Weber | PhD | Jamison |
| Bing Yan | PhD | Surendranath |
| Yoseob Yoon | PhD | Nelson |
| Yaqing Zhang | PhD | Nelson |

## Faculty Research Highlights

### Stephen L. Buchwald

The Buchwald Research Group's research focuses on the development of new methods for the formation of carbon-carbon and carbon-heteroatom bonds. The ability to make and modify compounds selectively allows access to a wide range of molecules that are important in the synthesis and design of pharmaceutical materials, agrochemicals, and natural products. In the past year, by studying mechanistic details, they designed a new ligand for copper-hydride catalyzed hydroamination. Using copper-hydride catalysis, they also found new methods to construct primary amines, $\alpha$-arylpyrrolidines, 1,2-diamines, indole derivatives, and tertiary alcohols. Additionally, they reported both milder and more robust techniques for the palladium-catalyzed and mediated carbon-nitrogen and carbon-sulfur cross-coupling reactions.

### Sylvia T. Ceyer

The Ceyer Research Group is exploring the role of spin in oxidation reactions of semiconductors as a fundamental dynamical principle critical to efficient oxidation at covalent solid interfaces. This project is being carried out using molecular beam–surface scattering techniques. In addition, a study into the acceleration of single-layer graphene growth on nickel by gold surface alloying continues, employing electron scattering as a vibrational spectroscopy for graphene detection.

### Arup K. Chakraborty

The Arup K. Chakraborty Group continued 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 harnessing for the rational design of vaccines and therapies is an important facet. Chakraborty, in collaboration with Professors Phillip Sharp and Richard Young, also continued to work on a project begun in 2016 on understanding how genes that are critical for maintaining healthy cell states are regulated. Their latest collaboration on this subject, published in 2018, was listed as one of the top 10 Breakthroughs of the Year by *Science* magazine. Chakraborty is also 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 continues to serve as a member of the US Defense Science Board and as a senior editor of *eLife* (one of the premier journals in biology). Chakraborty was awarded an honorary doctorate by the Hong Kong University of Science and Technology in 2019.

### Christopher C. Cummins

The Cummins Group synthesized and studied all-inorganic redox-active components for nonaqueous flow battery technology. Researchers also reported a new method enabling the use of orthophosphate and bisulfate as sources of value-added phosphorus and sulfur compounds, respectively. In an ongoing project using anthracene as a neutral leaving group, they showed that acyl(chloro)phosphines can be synthesized through phosphinidene transfer. This project also showcased anthracene as a launchpad for phosphinidene sulfide generation and for synthesis of a metastable semiconducting phosphorus–sulfur material. Finally, the group developed a novel triphosphorylating reagent for carbon, nitrogen, and oxygen nucleophiles.

### Rick L. Danheiser

In AY2019, the Danheiser Research Group completed the development of a new method for the chemical synthesis of pyridines, a class of organic compounds with applications in medicine, agriculture, and advanced materials. Researchers also completed the synthesis of furothienoindole, a unique tetracyclic molecule whose structure incorporates three different heterocyclic rings arrayed around a central benzene core. This synthesis featured the application of a powerful benzannulation strategy invented in the Danheiser laboratory.

### Mircea Dinca

In the past year, the Dincă Group has focused its efforts on creating new materials that tackle important environmental and energy challenges, including new solid electrolytes for batteries, more efficient ways to pump heat, and new materials for detecting ambient carbon dioxide levels. In these new developments, the group took advantage of researchers' knowledge in porous materials, which continue to be the fundamental focus of the group.

### Catherine L. Drennan

In AY2019, the Drennan Research and Education Laboratories employed X-ray crystallography to investigate the maturation of a nickel-iron-sulfur–containing metallocluster known as the C-cluster. The enzyme carbon monoxide dehydrogenase (CODH) employs this multi-metal cluster to oxidize carbon monoxide, removing an estimated $10^8$ tons of this pollutant from the environment every year. Little is known about how this metallocluster is assembled in nature. This lack has prompted the Drennan laboratory to investigate CODH expressed with and without a maturing enzyme CooC to determine the steps involved in cluster assembly.

### Robert W. Field

The Robert W. Field Group continues to focus on nitric oxide (NO)—a Goldilocks molecule. All of NO's Rydberg states accessible by 1- or 2-laser excitation from the ground state decay by rapid predissociation. A 3-laser scheme accesses long-lived *n*g Rydberg states (where "g" means an electron orbital angular momentum of four). It is easy to create a dense Rydberg gas of NO *n*g(v = 0) molecules; but at too high a density, fast decay by superradiance occurs. At v = 1, fast autoionization occurs. Nitric oxide is determined to keep its secrets, but it is no match for MIT spectroscopists.

### Robert Guy Griffin

The Griffin Group has developed a new technique, time optimized pulsed dynamic nuclear polarization (DNP) based on pulsed microwave irradiation. The technique should be useful for performing time domain DNP experiments at high frequencies and fields—800 megahertz for proton nuclear magnetic resonance (NMR) and 527 GHz for electrons. In a separate effort, group researchers determined that the so-called spin diffusion barrier around a paramagnetic polarizing agent does not really exist. This overturns a central pillar of the current understanding of the mechanism of DNP. In separate efforts, they continue to determine the structure of membrane proteins and amyloid fibrils. Their membrane protein efforts have focused on the voltage-dependent anion channel (VDAC) and amyloid fibrils associated with Alzheimer's disease.

### Mei Hong

In AY2019, the Hong Lab researchers:

1. Elucidated a 1.7 Å resolution structure of the amyloid fibrils formed by the peptide hormone glucagon. The peptide forms a novel antiparallel β-sheet with two coexisting molecular conformations. The solid-state NMR structure suggests strategies for designing glucagon analogs that inhibit fibril formation and improve the performance of this anti-hypoglycemia pharmaceutical compound.

2. Determined the three-dimensional fold and heterogeneous dynamics of the amyloid fibrils formed by the tau protein, which is involved in many neurodegenerative diseases, such as Alzheimer's disease. The study was the first time that both the molecular structure of the β-sheet core and the dynamics of the "fuzzy coat" domain of a full-length tau protein were characterized.

3. Solved the atomic (1.5 Å) structures of the closed and open states of the influenza B M2 proton channel. The two NMR structures gave novel insights into why protons are conducted in both directions by the influenza B M2 channel but only in the inward direction by the related influenza A M2 protein. This study was the first time that two states of an ion channel were structurally determined at such a high resolution in phospholipid bilayers.

4. Developed a novel, high-sensitivity $^{1}H$-$^{19}F$ distance NMR technique to measure interatomic distances up to approximately 2 nm. The technique is expected to be applicable to studying protein-ligand binding and membrane protein structure.

### Timothy F. Jamison

The Jamison Research Group, in collaboration with Klavs F. Jensen from Chemical Engineering, developed a fully integrated, reconfigurable, automated benchtop system for optimizing chemical reactions and producing laboratory-scale quantities of molecules. This system simplifies the labor-intensive chemical experimentation process, enabling researchers to focus their efforts on the more creative aspects of synthetic chemistry. The Jamison group also developed an automated continuous flow system capable of determining the concentration of highly reactive organometallic reagents used in chemical synthesis. This automated method is safer than, and demonstrates enhanced reproducibility over, standard procedures.

### Jeremiah A. Johnson

In the past year, the Johnson Research Group reported several advances in the synthesis and applications of functional polymers. In one study, they developed a new strategy for forming materials that can change their topology in response to light, thus allowing one material to exhibit the properties of multiple traditional materials. In another, they reported on the most sensitive organic (metal-free) magnetic resonance imaging (MRI) contrast agents known to date. These agents are promising as safer alternatives to metal-based MRI contrast agents. They also reported a new method for the functionalization of gold nanomaterials that significantly increases the stability of these systems, enabling their use in a variety of applications.

### Laura L. Kiessling

In AY2019, the Kiessling Lab developed a new way to examine the assembly of cell surface polysaccharides in bacteria. Laboratory members showed that bacteria process synthetic glycolipid substrates to build cell walls. These findings offer new ways to introduce unique functional groups into the bacterial polysaccharides that make up the cell wall, especially in mycobacteria, such as those that cause tuberculosis. The group anticipates that these groups can be used for imaging and for capturing glycans for drug screening, diagnosis, and vaccine generation.

In another project related to cell surface carbohydrates, laboratory members examined how dendritic cells (critical cells of the immune system) take up foreign antigens. They found that small soluble polymers decorated with sugars are taken up by dendritic cells and routed to compartments that degrade and process antigens. In contrast, particulate polymers (i.e., large insoluble aggregates) evade processing and are routed to the same compartments as human immunodeficiency virus (HIV). These findings highlight that the physical properties of HIV-1 are likely responsible for its trafficking in immune cells. The Kiessling Lab's studies provide inside into dendritic cell processing of antigens and guidelines for designing vaccines.

### Mohammad Movassaghi

The Movassaghi Group continues to focus on the development of new strategies and technologies for complex molecule synthesis. Group members recently reported the first enantioselective total syntheses of the complex alkaloid (+)-asperazine A through application of their biogenetically inspired electrophilic activation of cyclotryptophan substructures; this allows the revision of the sign and magnitude of the optical rotation for the reported structure. They also disclosed a detailed analysis of a permanganate-promoted oxidation of complex diketopiperazine substrates, a hydroxylation reaction developed in the laboratory that continues to serve as a critical transformation in the synthesis of anticancer epipolythiodiketopiperazine alkaloids. Group members continue to gain inspiration from nature in designing the chemical synthesis of complex molecules with high efficiency and stereochemical control in complex settings.

### Keith A. Nelson

AY2019 was an extraordinary year for the Keith Nelson Group, which reached several high-profile results. First, researchers demonstrated at far higher temperatures than previously a phenomenon called "second sound" in which heat travels in wavelike fashion rather than spreading out gradually as is usual. Their results offer hope that the phenomenon might be possible at room temperature or above, which would enable novel applications in nanoscale thermal management. In separate work, the group demonstrated "collective coherent control" over material structure. Researchers used low-frequency light to move atoms in a crystal directly into the positions they occupy in a new crystalline phase, thereby inducing a nonequilibrium phase transition. The dream of molecular coherent control, in which infrared light drives selected molecular stretching or bending vibrational modes whose motions lead directly to chemical reactions, proved unrealistic, but the collective version may be achievable in a wide range of materials.

### Elizabeth M. Nolan

The Nolan Lab demonstrated that the metal-chelating antimicrobial protein calprotectin inhibits iron uptake by diverse bacterial pathogens under aerobic conditions. In one case study, calprotectin induced iron-starvation responses in *Pseudomonas aeruginosa*. Analyses of the interplay between *P. aeruginosa* secondary metabolites—iron-binding siderophores and redox-cycling phenazines—and calprotectin indicated that ferrous ion withholding alters *P. aeruginosa* physiology and expression of virulence traits. This work is significant because it provides compelling evidence that calprotectin affects iron homeostasis and regulatory pathways in bacterial pathogens; it will thereby change working models for calprotectin's metal-withholding function.

### Bradley L. Pentelute

In AY2019, the Pentelute Lab leveraged bioconjugation strategies, intracellular delivery platforms, and rapid peptide synthesis technologies to optimize the production and function of a large variety of bioactive agents. Recent work revealed that cysteine arylation is a powerful avenue to chemically tailor unprotected peptides and proteins through both catalyst-free and palladium-mediated routes. These results were developed in an ongoing collaboration with the Buchwald group. The advantages imparted by these modifications were demonstrated by preparing potent macrocyclic antimicrobial peptides with improved serum stability, improving the affinity and stability of peptide-based inhibitors of cancer-specific protein-protein interactions, and endowing fluorine-rich cell-penetrating peptides with the ability to cross the blood-brain barrier. Researchers in the Pentelute laboratory also developed on-bead and in-solution platforms for the discovery of stable, non-immunogenic functional synthetic polymers composed of nonnatural D-amino acids. In the most recent development, machine-learning algorithms were applied to predict and improve the efficacy of cell-penetrating peptides. The goal is intracellular delivery of antisense oligonucleotides for the treatment of Duchenne muscular dystrophy.

### Ronald T. Raines

Ribonuclease is an enzyme that catalyzes the cleavage of RNA. In AY2019, the Raines Lab created a mouse that lacks extracellular ribonuclease; researchers found that this mouse formed blood clots too readily. This discovery suggests a natural role for ribonuclease in dissolving blood clots and the potential utility of exogenous ribonuclease as an anticoagulant.

### Alex K. Shalek

Cellular immunity is critical for controlling intracellular pathogens, but individual cell dynamics and cell-cell cooperativity in evolving human immune responses to infection have not been defined. In AY2019, the Shalek Lab developed a broadly applicable, high-resolution method that couples single-cell RNA sequencing with strategies for unbiased gene-module discovery to uncover distinct sets of cells responding in concert to complex stimuli over time. In collaboration with Dr. Bruce Walker's laboratory (Ragon Institute of MGH, MIT, and Harvard) and the laboratory of Thumbi Ndung'u (Africa Health Research Institute, KwaZulu-Natal, South Africa), Shalek laboratory members applied the method to profile, with unprecedented detail, the multicellular responses of four individuals before and immediately after untreated HIV-1 infection.

They were able to identify key populations of cells with potential effects on the course of the infection. Onset of viremia induced a strong interferon response across multiple lymphocyte and myeloid lineages. That response was followed by several cell-type-specific features, including pro-inflammatory T-cell differentiation, prolonged monocyte major histocompatibility complex-II upregulation, and persistent natural killer cell cytolytic killing. Longitudinal sampling revealed alignment of distinct cell-type-specific gene programs with viral load over time, implicating key intracellular- and extracellular drivers that induce them. Two of the four participants studied developed spontaneous viral control at late time points, associated with elevated frequencies of proliferating cytotoxic cells immediately after infection, inclusive of a previously unappreciated proliferating natural killer cell subset. Overall, the team's study provides a unified framework for characterizing the evolution of cellular responses at single-cell resolution. Its application to hyperacute HIV-1 infection highlights the importance of monocytes and natural killer cells in driving response coordination and possibly influencing the clinical trajectory, with prophylactic and therapeutic implications.

In parallel, through local, national, and international collaborations, the Shalek Lab pursued deep mechanistic inquiries across a diverse array of species and tissues, defining healthy compositions as well as deviations induced by different infections (e.g., *Mycobaterium tuberculosis*, HIV-1 and simian immunodeficiency virus, malaria, Ebola virus, hepatitis B, hepatitis C, and leprosy); inflammatory diseases (e.g., ulcerative colitis and Crohn's disease, psoriasis, alopecia, and granuloma annulare), and cancers (e.g., pancreatic and lung cancer, leukemia, and leptomeningeal disease) with a view toward novel therapeutic and prophylactic ends.

### Matthew D. Shoulders

The Shoulders Lab developed the first technique for continuous directed evolution in mammalian cells. A key limitation of traditional directed evolution workflows performed in test tubes, bacteria, or yeast is that these approaches yield products that very often fail to function when introduced into mammalian cells or organisms. Biomolecule functions evolved in simpler systems are often derailed in complex mammalian cells by off-target interactions, poor stability, or another problem. Previously, the only strategies for directed evolution in human cells involved screening of libraries generated by in vitro DNA mutagenesis or somatic hypermutation. These approaches are valuable, but they are also slow, inefficient, and afford limited library sizes. Members of the Shoulders Lab devised a system in which large mutational libraries are continuously generated in human cells, sophisticated selection schemes for many different biological activities continuously operate, and minimal experimenter intervention is required during directed evolution work. These advances have the potential to change how biotherapeutics are developed and optimized, as well as to open new doors in fundamental research in evolutionary biology.

### Yogesh Surendranath

The Surendranath Group aims to use electricity to rearrange chemical bonds by manipulating interfacial reactivity at the molecular level. Researchers have developed a molecular framework for understanding reactions of electrons and protons at electrode surfaces. They have developed a method for bypassing high-energy intermediates in molecular energy catalysis, and have found a way to use renewable electricity to convert methane into methanol.

### Timothy M. Swager

The Swager Group has once again produced major advances at the interface of chemistry, materials science, and technology. In the area of biosensors, group members have developed new methods for the detection of pathogenic bacteria; with the US Department of Agriculture, they performed field tests on the detection of *Salmonella enterica* contamination of chickens. These methods and related technology were the basis of a new Swager-founded start-up company, Xibus Systems. Swager has also initiated a program in membranes for separation and fuel-cell applications. In the area of gas separation, in collaboration with Professor Zachary Smith, group researchers have produced materials with record performance in separations of carbon dioxide, which is very relevant to energy technologies.

### Troy Van Voorhis

In the past year, the Van Voorhis Group made two major discoveries. First, group members showed that calculations on molecular systems can effectively be broken up into atom-based fragments using quantum embedding. Their results point the way toward revolutionary new ways of computing molecular properties in silicon. Second, they have shown that energy transfer between small semiconductor nanocrystals and molecules is governed by electronic states on the nanocrystal surface. Control of these surface states could yield improved solar energy technologies.

### Adam Willard

During AY2019, the Willard Group made research progress in several areas of theoretical and computational chemistry. They developed a new theoretical model and simulation platform for studying chemical reactions at electrode interfaces. These developments provided new insight into the role of the molecular interfacial environment in electrochemistry. In a separate effort, the Willard group developed a new theoretical framework for studying population dynamics of open quantum systems that enables the straightforward application of classical methodologies to inherently quantum problems.

### Bin Zhang

The Zhang Group developed an information theoretic model to infer the formation mechanism of domain-level chromatin states from genome-wide epigenetic modification profiles. Group members also developed a polymer model to enable de novo prediction of chromatin organization at 5 kilobase resolution. In addition, they have established a collaboration with Bradley Bernstein from the Broad Institute to model whole-genome organization and to investigate genome misfolding on tumorigenesis. They are also working with James Liu from the Howard Hughes Medical Institute to apply a super-resolution imaging technique to determine spatial localization of accessible chromatin at a genomic scale for individual cells.

**Stephen L. Buchwald**
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