Department of Chemistry

In academic year 2021 (AY2021), the Department of Chemistry had 31 full-time faculty, one dual faculty appointment with Institute for Medical Engineering and Science (IMES): five assistant professors, three associate professors without tenure, four associate professors with tenure, and 19 full professors. Six additional faculty members—Arup K. Chakraborty (Robert T. Haslam (1911) Professor in Chemical Engineering, professor of Physics, and core faculty of IMES), Catherine L. Drennan (professor of Biology), Barbara Imperiali (Class of 1922 Professor and professor of Biology), Susan Solomon (Lee and Geraldine Martin Professor in Environmental Studies, professor of Atmospheric Chemistry and Climate Science), Steven R. Tannenbaum (Underwood-Prescott Professor Post-Tenure and professor post-tenure of Toxiocology and Biological Engineering), John M. Essigmann (William R. (1956) and Betsy P. Leitch Professor in Residence and professor of Toxicology and Biological Engineering)—have secondary appointments in Chemistry. Robert Field, Robert T. Haslam and Bradley Dewey Professor and professor of Chemistry, transitioned to professor post-tenure starting July 1, 2021. In addition to research in biological, inorganic, organic, materials and nanoscience, organic, physical, and computational and theoretical chemistry, the department continued its strong programs in undergraduate and graduate education, with 248 graduate students, 103 postdoctoral researchers, and 69 undergraduate chemistry majors.

Bradley L. Pentelute, professor of Chemistry, was promoted to full professor; Alexander T. Radosevich, associate professor of Chemistry, and Alex K. Shalek, associate professor of Chemistry and core faculty of IMES, earned tenure; and Bin Zhang, Pfizer Laubach Career Development Professor, was promoted from assistant professor of Chemistry to associate professor without tenure, effective July 1, 2021. Brett McGuire joined the faculty as assistant professor of Chemistry, and the department welcomed Danna Freedman, Frederick George Keyes Professor, from Northwestern University. Alex M. Klibanov, Novartis Professor announced his retirement, and transitioned to professor emeritus.

Highlighted Faculty Awards and Honors

In August, McGuire was named one of Chemical & Engineering News' Talented 12, which highlights early-career researchers in the chemical sciences who are fearlessly tackling difficult global problems.

In August, Mei Hong, professor of Chemistry, won the 2021 Nakanishi Award from the American Chemical Society. Sponsored by the Nakanishi Prize Endowment, this award is given in recognition of application of spectroscopy to biological phenomena.

In November, Drennan was elected a Fellow of the American Association for the Advancement of Science on honor of her effort to advance science.

In December, Gabriela Schlau-Cohen, associate professor of Chemistry, won the 2021 Marion Milligan Mason Award. This biennial award is given in support of the advancement of women in the chemical sciences.

In December 2020, Timothy M. Swager, John D. MacArthur Professor and professor of Chemistry, was elected to the National Academy of Inventors, the highest professional distinction accorded solely to academic inventors.

In February, Keith Adam Nelson, Robert T. Haslam and Bradley Dewey Professor and professor of Chemistry, received the 2021 William F. Meggers Award from The Optical Society of America (OSA). The OSA Awards Program celebrates the field's technical, research, education, business, leadership and service accomplishments.

In April, Pentelute received the 2021 Rao Makineni Lectureship. This lectureship, given biennially, honors Rao Makineni, a long-time supporter of peptide science, peptide scientists, and the American Peptide Society.

In April, Robert G. Griffin, Arthur Amos Noyes Professor and professor of Chemistry, was elected to the National Academy of Sciences. He was one of 120 new members elected in recognition of their distinguished and continuing achievements in original research.

In April, Drennan was named an American Society for Biochemistry and Molecular Biology (ASBMB) Fellow. She is a member of the inaugural class of ASBMB Fellows honored for their efforts to advance the molecular life sciences.

In April, Shalek won the 2021 Avant Garde Award from the National Institute on Drug Abuse. This award is given annually in recognition of the exceptional creativity of those who propose high-impact science that will open new areas of HIV research.

In May, Rick Lane Danheiser, Arthur C. Cope Professor and professor of Chemistry, was named the recipient of the 2021 Gordon Y. Billard Award by MIT. This award is given annually in recognition of an individual's service of outstanding merit to the Institute.

In June, Mircea Dincă, W. M. Keck Professor of Energy and professor of Chemistry, was named a 2021 Blavatnik Award Finalist. Blavatnik Scholars are recognized for their contributions to the advancement of the human condition through scientific progress.

Fundraising

Fundraising from individuals and private foundations remains a priority for the department. Chemistry was able to have a very successful year in spite of the pandemic. We hosted events and faculty talks for alumni, parents, and friends virtually that allowed donors of the department to stay connected.

The department successfully had its second best fundraising year in the last five years. New gifts and pledges to Chemistry in fiscal year 2021 (FY2021) totals $3.72 million—a 177% increase from FY2020. The increase was largely due to the influx of planned gifts, major gifts, and foundation gifts. We saw our biggest increase in the $100,000 to $499,000 range and it is our goal to continue to cultivate donors in this critical giving band. As we look ahead, Chemistry's top fundraising priorities will continue to be fellowships, the Chemistry Discretionary Fund, and laboratory renovations. We are excited to join forces with our partners in Resource Development and the Alumni Association to increase the department's donor pipeline and to foster those relationships already created.

Named Lectures

Due to the COVID-19 pandemic, there were no named lectures held in the fall of 2020 or the spring of 2021.

Serving the Institute

The Department of Chemistry provides key educational service to the Institute. During AY2021, the Department of Chemistry taught 1,193 MIT undergraduate students in the areas of biochemistry, inorganic, organic, and physical chemistry.

Even with the challenges of the COVID-19 pandemic and many students enrolling remotely for all or part of the year, the Undergraduate Research Opportunity Program (UROP) continued to thrive. The department was the home for 57 UROP students providing important mentoring relationships for students from a number of departments, including chemistry, biology, physics, brain and cognitive science, chemical engineering, and biological engineering.

Chemistry Majors

We continue to consistently attract a very talented group of undergraduates to Courses 5 and 5-7, with a total of 69 majors across the three years, 28 in Course 5, and 41 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. Under the ChemFlex Option, 11 students have graduated so far, and 14 students are currently pursuing the option as sophomores and juniors. Examples of our students' focus areas include Organic Material Science, Computational Chemistry, Neuroscience, and Science Education.

This year, 17 students received SB degrees in Chemistry, 6 in Course 5 (5 with the ChemFlex Option) and 11 in Course 5-7. Based on self-report, 35% of the Class of 2021 will be attending a PhD program, 18% will be attending an MD/PhD program or medical school, and 35% will be working. Post-MIT plans for 12% of the students were unknown.

Undergraduate Research Opportunity Program

UROP continues to be the capstone experience for our undergraduates. Every member of the Class of 2021 worked in a research group at least once during their degree program. This year one of our graduating seniors, Agata Bikovtseva, received the 2021 Outstanding UROP Student Award—School of Science. This award, given annually by the Institute, recognizes MIT undergraduates who have made outstanding commitment, and significant contribution, to research in their field. Looking at the Class of 2022 and Class of 2023, 83% have worked in a research group at least once so far. Our undergraduates have the unique opportunity to conduct research alongside faculty, postdoctoral researchers, and graduate students.

Chemistry Teaching Assistants

Our graduate student teaching assistants (TAs) are some of the best at MIT. The Chemistry lab TAs did an amazing job with their in-person teaching responsibilities; they are always very focused on safety and this year there was the extra challenge of carefully following all of the COVID-19 pandemic-related protocols. The lecture TAs were also outstanding, providing remote instruction and support to all of the students taking Chemistry subjects. This was all accomplished while the TAs themselves were taking classes remotely and adjusting to graduate school in the midst of the pandemic.

Undergraduate Awards

The Department of Chemistry recognized recipients of Undergraduate Awards during the 2021 virtual celebration of Commencement on June 3, 2021.

First-Year Chemistry Achievement Award

For outstanding academic achievement in chemistry:

- Ana Florescu-Ciobotaru
- Shicheng Hu
- Cholapat Varongchayakul

Outstanding Sophomore Achievement Award

For outstanding achievement in academics, research, and service to the Department of Chemistry:

- Vinicius Armelin

Outstanding UROP Presentation Award

For outstanding undergraduate research and in recognition of the best presentation at the 2021 Chemistry UROP Symposium:

- Alby Joseph

Alpha Chi Sigma

For outstanding achievement in scholarship, research, and service to the Department of Chemistry:

- Harrison Wang

Research

For outstanding contributions in the area of research:

- Agata Biovtseva
- Ameena Iqbal
- Dayanne Rolim Carvalho
- Rachel Weissman

Royal Society of Chemistry Certificate of Excellence

For outstanding scholarship:

- Zhengkai Huang
- Alby Joseph
- Anna Khoroshilov
- Eleane Lema
- Siam Muquit
- Deborah Wen

Service

For significant contributions in the area of service to the Department of Chemistry:

- Siam Muquit
- Miller Tan

Phi Beta Kappa 2021 Inductees

- Zhenkai Huang
- Alby Joseph
- Anna Khoroshilov
- Eleane Lema
- Siam Muquit
- Harrison Wang
- Deborah Wen

Teaching Assistant Awards

- Ezra Alexander
- Alison Biester
- Bella Borgula
- Sam Detmer
- Andrei Iliescu
- Alayna Johnson
- Jess Kim
- So Young Lee
- Wei Hao Lee
- Kunal Lodaya
- Linsey Nowack
- Jules Oppenheim
- Yanina Pankratova
- Robert Raclea
- Greg Schuette
- Madi Scott
- Xin Sui
- Jiakun Tian
- Leah Weisburn

Excerpts from TA Evaluations for Fall 2020 and IAP 2021

"… was incredibly supportive and responsive throughout the semester, which I really appreciated in a remote context. He accommodated feedback about recitations and teaching format throughout the term, and was a joy to learn from, as a person and as a TA :)"

"… was such an amazing TA!! Her enthusiasm for chemistry was infectious and made the material much more interesting. I also know that she put hours into making our recitation slides every week and making practice problems. She always went above and beyond and sent us clarificatory emails about questions that were asked in class. If she could not answer a question immediately, she would always find the answer and get back to us. Her office hours were also super helpful. I definitely would not have survived this class without her!"

"… was one of the best TAs I have had so far. He went beyond my expectations by staying after recitation to help anyone who needed it, by stimulating our desire to learn by providing concrete parallels and additional information whenever relevant, and by leading expert recitations that prepared us well for exams among many others."

"Great teaching skills! I liked the ways … explained the key concepts during recitations and it helped me a lot in systematizing my knowledge for the exams. Additionally, the review sessions before the exams addressed students' specific questions and only added to my further understanding of the material."

"… is one of the best TAs I've had at MIT. He was always warm to questions or concerns and he genuinely cares about chemistry. It also felt like he cared about how each of the people in his recitation were doing. He showed a strong understanding of chemistry and was able to help me learn effectively."

"My favorite TA I've ever had across multiple departments at MIT. Her office hours were good because she did not just give the answer but rather asked the students questions for them to arrive at the answer on their own. Was not really looking forward to OChem coming into this semester but I really enjoyed the class, and she's the main reason why. Please let her TA for 5.13 :)"

"… was the best TA by far!! I really appreciated him going out of his way to include everyone in conversations, give us extra information pertinent to the labs, and his thorough knowledge of the material."

Doctoral and Master's Degree Recipients

Doctoral degree recipients in September 2020:

- Odin Achorn, Bawendi Group
- Kenny Chen, Shoulders Group
- Krysta Dummit, Radosevich Group
- Alethe Gaillard de Saint Germain, Shalek Group
- Jordan Ho, Kiessling Group

- Rebecca Holden, Pentelute Group
- Alexander Hull, Field Group
- Henry Kilgore, Raines Group
- Austin Kruger, Kiessling Group
- Alexander Loftis, Pentelute Group
- Anna Ponomarenko, Shoulders Group
- Anthony Quartararo, Pentelute Group
- Minjung Son, Schlau-Cohen Group
- Cassandra Zentner, Swager Group

Doctorial degree recipients in February 2021:

- Roger Diehl, Kiessling Group
- Christine Isabella, Kiessling Group
- Corey Kaminsky, Surendranath Group
- Venkata "Shiva" Mandala, Hong Group
- Dmitro Martynowych, Nelson Group
- Thanasak Sathitwitayakul, Ceyer Group
- Timothy Sinclair, Bawendi Group
- Yujing Zhou, Buchwald Group

Doctoral degree recipients in June 2021:

- Daniel Banks, Griffin Group
- Gregory Cleveland, Radosevich Group
- Jesús Dones-Monroig, Raines Group
- Yi "Frank" Gao, Nelson Group
- Martin Gelenter, Hong Group
- James "Connor" Gilhula, Radosevich Group
- Ryan King, Buchwald Group
- Aaron Mallek, Buchwald Group
- Katie McGeough, Jamison Group
- Jonathan Melville, Surendranath Group

- Hye Won "Hanna" Moon, Radosevich Group
- Zachary Nelson, Swager Group
- Jiaojian "Tristan" Shi, Nelson Group
- Yuchen Sun, Nelson Group
- Erica Tsai, Buchwald Group
- You-Chi "Mason" Wu, Swager Group
- Kristin Zuromski, Baker Group

Master's degree recipients in June 2021:

- Johanna Barbour, Wendlandt Group
- Daniel Harper, Kulik Group
- Carolyn Suh, Wendlandt Group
- Kathleen Wang, Wendlandt Group

Due to the COVID-19 pandemic, the department held what will hopefully be the final virtual Commencement and Investiture of Doctoral Hoods/Degree Conferral ceremonies in June of 2021. The graduates of 2021 were celebrated with a Virtual Graduation Celebration held via Zoom on June 2 (for Masters and PhD recipients) and June 3, 2021 (for undergraduate recipeints). 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, in addition to students' advisors and/or mentors.

Visit the Chemistry website for a recap of the Virtual Investiture of Doctoral Hoods and Degree Conferral Ceremony.

Faculty Research Highlights

Stephen L. Buchwald

The Buchwald research group focused on the development of new methods for the formation of carbon-carbon and carbon-heteroatom bonds. In the past year, the group:

1. devised new transformations using copper-hydride catalysis for the synthesis of b-chiral amides, a-chiral carboxylic acids, functionalized benzimidazoles and used dual copper-hydride and palladium catalysis for the synthesis of a-chiral olefins;
2. invented new general palladium catalyst systems to access a broad scope of aryl amines; and
3. in collaboration with Pentelute's group, used palladium reagents for selective biofunctionalization of proteins, peptides and oligonucleotides.

Jianshu Cao

Microscopic objects such as photons, 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. In AY2021, the Cao group studied quantum coherence in light-harvesting complexes, organic aggregates, molecular junctions, and optical cavity systems, 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

Unlike the surface of pure Ni metal, a surface of Ni-Au alloy catalyzes the growth of graphene nanoflakes under low temperature conditions. The role of bulk C in this growth is being explored. In a second project, van der Waals dimers are being used to probe the nature of spin transitions in the oxidation of covalent solid interfaces using molecular beam-surface scattering techniques.

Christopher C. Cummins

The Cummins lab reported the synthesis, structure, and nickel complexation of an anthracene-based macrocyclic diphosphine ligand. The group reported the synthesis and structural characterization of the first 3,5-diphenyl-2-phosphafuran, a Diels-Alder diene capable of undergoing thermally reversible [4 + 2] cycloaddition with unactivated olefins, including ethylene. Also developed was methodology for the preparation of α,δ-disubstituted tetraphosphates and terminally functionalized nucleoside pentaphosphates. Together with collaborators Mei Hong and Daniel Nocera, Patterson Rockwood Professor of Energy at Harvard University, the group showed that bacterial phosphate granules contain cyclic oligophosphates in addition to the already appreciated linear ones. They showed that the molecular form of P_2O_5 can be stabilized using simple N-donor ligands.

Mircea Dinca

The Dincă group has made important steps to understand and control the growth of series of new two-dimensional electronic metal-organic framework (MOF) materials known as conductive 2D MOFs. These have applications in energy storage and conversion. In a parallel line of research, we have provided conclusive evidence for the existence of elusive, reactive species such as hyponitrite, involved in the industrial NOx reduction chemistry and in biological signaling.

Catherine L. Drennan

Acetogenic organisms can grow on CO_2/H_2 through the Wood-Ljungdahl pathway and action of carbon monoxide dehydrogenase/acetyl-CoA synthase (CODH/ACS), which catalyzes the reduction of CO_2 to CO at a Ni-Fe-S-containing metallocofactor called the C-cluster, and catalyzes the condensation of CO, CH_3^+, and CoA to acetyl-CoA at a

Ni-Fe-S-containing metallocofactor called the A-cluster. In the past year, the Drennan lab published the first crystal structure of a substrate-bound state of the A-cluster: the carbonylated state.

John Essigmann

In August 2021, John Essigmann will be awarded the Founders' Award of the Division of Chemical Toxicology at the American Chemical Society Meeting in Atlanta. The reward reflects his career-long study of the structural and genetic effects of specific types of DNA damage, especially DNA damage caused by chemical carcinogens, ionizing radiation and chemotherapeutic agents. Essigmann's most recent work identified high-resolution mutational patterns in human liver and brain tumors that reflect prior exposure to chemical carcinogens.

Robert W. Field

When a diatomic molecule is excited to an energy higher than its Ionization limit, it needs to decide whether to split into two atoms or spit out an electron. These two processes are so tangled up for the NO molecule that, for 50 years, no experiment has given a clear picture of the microscopic mechanism of either process. The Field Group has shown that, by exciting one electron to high angular momentum, a centrifugal barrier prevents the electron from transferring its energy into its ion-core by a hard dissociating collision. The electron interacts with the not-round ion-core and gains its freedom by an energy and angular momentum exchange in which the microscopic mechanism is encoded in the correlated angular momenta of the departing free ion and free electron.

Robert Guy Griffin

High frequency dynamic nuclear polarization (DNP) is conventionally performed using a gyrotron to generate continuous-wave microwaves. Pulsed DNP has only been demonstrated at lower fields where high power microwave sources are readily available. Performing the DNP experiments at higher-fields requires microwave instrumentation capable of producing arbitrarily shaped high-power pulses. Pulse shaping is easily achieved using a commercial arbitrary waveform generator and standard solid-state components operating initially at lower powers. Here, the Griffin Group has demonstrated an advance in microwave technology enabling conversion to 250 GHz with a relatively high output power of 250 mW. The power is adequate to excite Overhauser effect (OE) DNP enhancements, and they used the apparatus to investigate OE-DNP in a variety of 1,3-bisphenylene-2-phenylallyl (BDPA) variants. An enhancement ε ~70 was observed for the Overhauser effect in the bulk ^{1}H in BDPA at 90 K and at a MAS rate of 5 kHz.

Mei Hong

The Hong laboratory accomplished several highly impactful studies of infectious disease proteins, including a SARS-CoV-2 protein and an antibiotic-resistant protein. These timely studies have been widely reported in the news media. They also conducted cutting-edge studies of an amyloid protein that is critical in many neurodegenerative diseases.

- The Hong group reported the atomic-resolution structure of an essential membrane protein of the SARS-CoV-2 virus, the causative agent of COVID-19.
- The Hong group solved a long-standing structural biology puzzle by reporting the high-resolution structure of a bacterial transporter, EmrE.
- The Hong group investigated the three-dimensional structure of a full-length tau protein, which is involved in many neurodegenerative diseases such as Alzheimer's disease.

Timothy F. Jamison

The Jamison group, in collaboration with Klavs F. Jensen, Warren K. Lewis Professor of Chemical Engineering and professor of Materials Science and Engineering, developed a fully-integrated, self-reconfiguring robotic system that designs and carries out molecular synthesis in an automated fashion. This system includes a machine learning approach developed in the course of this collaboration that designs syntheses with an expertise and accuracy comparable to that of advanced undergraduates and beginning graduate students. Together 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 reported a new strategy to enable on-demand degradation and recycling of a class of materials called thermosets, which represent approximately 20% of plastic and rubber used today and cannot be recycled. Additionally, we introduced a new prodrug platform for the safe and effective delivery of bromodomain and extra-terminal protein inhibitors with applications in triple negative breast cancer therapy. Finally, we disclosed a novel liquid electrolyte formulation that enables stable lithium-metal batteries, offering potential to double the energy density of batteries used today in portable electronic devices and electric vehicles.

Brett McGuire

This year, the McGuire group opened a brand new window into humanity's understanding of the cosmic evolution of carbon. Using laboratory chemistry and observational astronomy, the group detected individual polycyclic aromatic hydrocarbon molecules in space for the first time. These molecules are thought to contain as much as a quarter of all carbon in space, making them perhaps the most critical window into how carbon cycles through the process of forming stars and planets.

Mohammad Movassaghi

The Movassaghi Lab continues to focus on the development of new strategies and technologies for complex molecule synthesis. They recently disclosed a previously unappreciated interaction that leads to stabilization of the disulfide bond in epidithiodiketopiperazine alkaloids, a large class of anticancer compounds that my group has investigated for over a decade. They conducted a physicochemical study to evaluate the energetic contribution of this interaction to stabilize their structure

and determined how this may contribute to their potent anticancer properties. The group also reported on the direct sulfidation of amides via electrophilic activation and use of sulfoxide reagents as nucleophiles to give alpha-sulfide amide products. They continue to gain inspiration from nature in designing our chemical synthesis of complex molecules with high efficiency and stereochemical control in complex settings.

Keith Nelson

The Nelson group made new progress in methods for optical control and observation of materials under far-from-equilibrium conditions. They demonstrated new ways to use pulsed laser light to generate strong mechanical shocks and strong terahertz-frequency electromagnetic waves whose electric fields could drive excursions into new molecular and collective states. They also conducted real-time observations of transition metal dichalcogenide samples during their far-from-equilibrium transitions into new collective electronic and structural states. The combination of optical control over large-amplitude motions away from equilibrium and single-shot optical observation of irreversible processes opens a direct window onto the pathways and dynamics of collective material transformations.

Elizabeth M. Nolan

The Nolan Lab continued to investigate the metal-sequestering innate immune function of S100 proteins, including calprotectin (CP), and antimicrobial siderophore-antibiotic conjugates that target bacterial iron-uptake machinery. In one particular initiative, the effect of heme, the most abundance iron source in humans, on the response of *Pseudomonas aeruginosa* and *Staphylococcus aureus* to iron-withholding by calprotectin was examined. This study revealed that CP causes both bacterial pathogens increase expression of heme transport machinery, and that both species will use heme as a nutrient iron source and thereby overcome iron-withholding by CP. This work is significant because it is the first examination of how a biologically relevant iron source affects bacterial responses to metal withholding by calprotectin and suggests how these pathogens will adapt to avoid iron starvation induced by calprotectin.

Bradley L. Pentelute

There are more amino acid permutations within a 40-residue peptide sequence than there are atoms on Earth. This vast chemical search space hinders the use of human learning to design functional peptides. This past year, the Pentelute Group coupled supervised and unsupervised deep learning with high-throughput experimentation to drive the discovery of peptides that deliver antisense oligonucleotide to the nucleus of cells. The new peptides boosted activity by 50-fold, are effective in animals and are nontoxic. Machine learning can discover functional peptides that enhance cellular uptake of potential therapeutics.

Alexander T. Radosevich

In the past year, the Radosevich Lab discovered several new aspects of reactivity at low-symmetry phosphorus compounds. An organophosporus-catalyzed procedure for reductive C-N coupling of nitromethane and arylboronic acids to give N-methylanilines was reported. A phosphorus(II) tiamide was found to support catalytic arene borylation

and stoichiometric arene dehydrofluorination reactivity. The application of such nontrigonal phosphorus(III) triamides as nonspectator ligands for transition metals resulted in the report of a novel alkyl migration reaction.

Ronald T. Raines

Boron sits next to carbon in the periodic table and has many useful properties. Yet, only five FDA-approved drugs contain boron. The reason for this striking underutilization is the instability of boron to oxidative damage. The Raines Group discovered a context in which boron retains its desirable attributes but is 10,000-fold more stable to oxidation. This new functional group has utility in chemistry, biology, and medicine.

Alex K. Shalek

There is a pressing need to understand the pathogenesis of the severe acute respiratory syndrome coronavirus clade 2 (SARS-CoV-2) responsible for the COVID-19 pandemic. This year, the Shalek Lab, in collaboration with several researchers around the world, leveraged single-cell/nucleus RNA-sequencing (sc/snRNA-seq), highly multiplexed spatial imaging, flow cytometry, and other methods to define the primary cellular targets of SARS-CoV-2 and how COVID-19 impacts respiratory tissues. In one study, by examining cells collected from nasopharyngeal swabs, they discovered that COVID-19 dramatically alters the composition of the nasal epithelia, and that individuals who go on to have more severe disease display early defects in intrinsic epithelial antiviral responses (Ziegler et al, *Cell*, 2021). In another, by characterizing autopsy donor tissue samples, they similarly uncovered substantial remodeling of the lung epithelial, immune, and stromal compartments in severe disease, with evidence of multiple failed attempts at epithelial tissue regeneration (Delorey et al, *Nature*, 2021). In both, they resolved cells harboring viral transcripts, and identified genes likely involved in susceptibility, resistance, or infection response. Collectively, these and related studies reveal detrimental as well as protective cell and tissue level responses to SARS-CoV-2. Further, they suggest that failed epithelial cell behaviors may underlie and predict severe COVID-19.

In parallel, through local, national, and international partnerships, the Shalek lab pursued deep, mechanistic inquiry to elucidate the cellular and molecular features that inform tissue-level function and dysfunction across the spectrum of human health and disease (infectious: tuberculosis, HIV-1, ebola, leprosy, malaria, environmental enteropathy; inflammatory: ulcerative colitis and Crohn's, psoriasis, alopecia, granuloma annulare; and cancer: pancreatic, breast, colon, and lung cancer, B-Acute Lymphocytic Leukemia, melanoma, and leptomeningeal disease), to aid in the design of therapeutic and prophylactic interventions to improve human health.

Matthew D. Shoulders

The Shoulders Lab in the Department of Chemistry solved a decades-old biochemical mystery, discovering why sugars (N-glycans) are installed on the second-most abundant protein in the world—collagen. In brief, the sugars serve as an essential safeguard promoting the folding and production of collagen under stressful conditions such as those encountered during wound-healing or development. Among other advances, they also established a new strategy to address disease-causing collagen misfolding by targeting the collagen proteostasis network.

Daniel L. M. Suess

The Suess group characterized dinitrogen binding to clusters of iron and sulfur atoms that serve as models of the active site of nature's catalyst for converting dinitrogen to ammonia: nitrogenase. They also discovered and reported a method for manipulating the composition of these and related iron-sulfur clusters. The group's method affords precise control over the placement of isotopes in specific iron sites and thereby yields new insights into the spatial distribution and coupling of electrons in these clusters.

Yogesh Surendranath

The Surendranath group aims to use electricity to rearrange chemical bonds by manipulating interfacial reactivity at the molecular level. The group has developed new molecular metal complexes that model the active sites in earth-abundant fuel cell catalysts. They have developed a mechanistic understanding of the partial electrochemical oxidation of methane to methyl esters. They have developed general methodologies for using interfacial electric fields to control thermochemical catalysis.

Timothy M. Swager

The Swager group invented a new generation of methane sensor that is inexpensive, low power, and highly sensitive. The sensor responds to part per million (ppm) concentrations of methane and provides a change in electrical resistivity as its output. Methane is a far more problematic green house gas than carbon dioxide. This new technology can be used to detect trace methane emissions that are an increasing contributor to climate change.

Troy Van Voorhis

The Van Voorhis group has made exciting new discoveries concerning the surface electronic structure of nanoscale crystals of semiconductors, also known as quantum dots. These tiny objects are at the heart of cutting edge display and lighting technologies and our results reveal that the electrons at the surface of these structures behaves in unexpected ways—creating a myriad of surface defects that dominate the photochemistry of these systems.

Xiao Wang

The research of Wang Lab focuses on developing and applying state-of-the-art chemical and biological tools to understand molecular events underlying tissue architecture and function. In the past year, we have developed an integrative computational approach to analyze spatial gene expression as well as experimental methods to measure single-cell gene expression and electrophysiology simultaneously in the mouse brain, enabling high-throughput discovery of key molecular pathways in tissue function.

Adam Willard

The Willard Group made several advances in the areas of molecular quantum computing, theoretical electrochemistry, and protein hydration. Working with the Schlau-Cohen and Bathe groups, we developed a theoretical platform for engineering physical systems of precisely arranged dye molecules that upon illumination are

capable of performing rudimentary quantum computations. With this platform we have designed systems that can carry out the universal quantum gate operations. In the area of of electrochemistry, we have carried out simulations of the molecular scale properties of electrochemical interfaces, such as those implicated in many renewable energy applications. With the Manthiram group we have developed a Bayesian approach to improved parameter estimation from electrochemical experience. In the area of protein hydration, we are working on utilizing the tools of machine learning to identify ligand binding sites on proteins based only on the molecular signatures of the surrounding water layer. This advance may contribute to more efficient and robust methodology in computer-aided drug design.

Bin Zhang

The Zhang Group has taken an integrative approach to study whole-genome organization by utilizing data from various experimental techniques. They revealed a remarkable change in genome organization upon tumorigenesis. In addition, the group found that the chromatin network contributes to the stabilization of a multi-droplet state. This mechanism succeeds at explaining the co-existence of multiple nucleoli and the increased number of nucleoli in cancer.

Troy Van Voorhis
Department Head
Haslam and Dewey Professor of Chemistry