Department of Chemical Engineering

Overview

During academic year 2021, the Department of Chemical Engineering continued its long tradition of global leadership in the discipline. For the 30th straight year, our undergraduate and graduate programs were each ranked number one by *US News & World Report*. The department was also ranked first in the QS World University Rankings for chemical engineering for the seventh consecutive year and contributed to the record-breaking 10th straight year that MIT was ranked first among world universities overall. The department continues to maintain its reputation and record of excellence at a time of increasing competition, investment, and growth among chemical engineering programs at peer institutions.

With the completion of both our task force on undergraduate curriculum revitalization and our regularly scheduled review with the Accreditation Board for Engineering and Technology (ABET) last year, our undergraduate program focus shifted toward ensuring continuous assessment and improvement. We modified requirements for the non-accredited 10C degree to align with previously implemented changes for ABET-accredited Courses 10, 10B, and 10-ENG, and we established a formal schedule for a regular review of core courses. Following a focus group with 10-ENG seniors, the department established a certificate process to recognize each graduate's chosen concentration. The department also continued its partnership with the Department of Biological Engineering in operating the Huang-Hobbs BioMaker Space. This innovative project leverages national trends in mechanical and electrical makerspaces to empower undergraduates in experimenting with biological and chemical design while providing a home to a new community of undergraduates connected through the BioMaker Club.

The department expanded its leading efforts in developing and following best practices to promote equity and inclusion in all of our actions and activities. The new Diversity, Equity and Inclusion (DEI) Committee was formally launched within the last academic year under the direction of faculty and staff co-leads (Professor Chris Love and Sharece Corner, respectively) and includes additional faculty and staff, undergraduates, graduate students, and postdoctoral associates. In forming this committee, the department's goals are to engage all constituencies in these important matters and to establish a long-lasting mechanism to ensure that our commitment does not waver or wane. The DEI Committee complements the work of our two graduate student programs: the ChemE Application Mentorship Program, which mentors students on applications to our graduate program, and the Diversity in Chemical Engineering Program. The department continues to host the ACCESS program, a weekend of educational and informative events introducing talented sophomores, juniors, and seniors to the benefits of a graduate education in chemistry, chemical engineering, and materials science. The required virtual nature of ACCESS this past fall enabled expanded participation through an open application process. Three former ACCESS participants are currently matriculating in the doctoral program; one student, Gabriel Sanchez-Velazquez, will arrive in fall 2021. The department also virtually hosted its third Rising Stars in Chemical Engineering Workshop, which is aimed at preparing women for the challenges associated with a career in academia. One of two new faculty recruits, Qin "Maggie" Qi, is an alumna of the Rising Stars program.

The department continues to attract significant research funding at an annual volume of $50.9 million, of which $21.4 million is handled directly through the department; the remaining funds are managed by various other cost centers at MIT. Faculty members continue to secure healthy funding for their individual research programs while participating in the creation and direction of larger multi-investigator projects. Chemical Engineering faculty also continue to lead large, multi-institutional research centers, as further explained below.

Our faculty, students, and staff continued to respond to the impact of the Covid-19 pandemic during the past academic year. With only seniors in residence in the fall, the teaching labs (10.28 Chemical-Biological Engineering Lab and 10.467 Polymer Science Lab) were the only courses in the undergraduate curriculum offered in person. The spring term featured in-person labs and hybrid core courses, with lectures conducted remotely and small group recitations offered in person. The hybrid model was also employed for first-year graduate core courses. The department has benefited greatly from the exceptional service of the staff of the infrastructure team (Robert Fadel, Jim Hardsog, Chris Monaco, Brian Smith, and Gwen Wilcox) throughout these trying times.

Professor Paula T. Hammond completed her sixth year as department head, while Professor Kristala Prather is in her second year of service as executive officer. Professor Patrick Doyle continued to serve as graduate officer, and Barry Johnston continued his long service as undergraduate officer. Professor Bill Green completed his sixth year as postdoctoral officer, and Professor Martin Z. Bazant completed his first as the inaugural digital learning officer. Professor T. Alan Hatton remains the director of the David H. Koch School of Chemical Engineering Practice. Professor Robert Armstrong is the director of the MIT Energy Initiative (MITEI). With this year's recognition of Paula Hammond and Arup Chakraborty, Chemical Engineering now has three Institute Professors as primary faculty members (the other being Robert S. Langer). The department mourned the loss of faculty member and Institute Professor Daniel I.C. Wang this past fall.

New Arrivals and Promotions

The department recruited two faculty in FY2021: Professors Brandon Dekosky and Maggie Qi. This year, Professors Kwanghun Chung, Heather Kulik, and James Swan all received tenure promotions. In addition, two of our senior faculty members, Arup K. Chakraborty and Paula T. Hammond, were named Institute Professors.

The department welcomed two new staff members: Robert D. Fadel from MIT's Center of Excellence for Energy joined as the department's administrative officer, and Leposava Gagoska from MITEI joined as a financial coordinator.

Research and Recognition

Many members of the Chemical Engineering faculty received major awards for their research and related teaching achievements. Ariel Furst earned an MIT Abdul Latif

Jameel Water and Food Systems Lab (J-WAFS) seed grant to detect and degrade pesticides. Katie Galloway received a National Institutes of Health (NIH) Maximizing Investigators' Research Award. Emeritus Professor Karen Gleason won the American Institute of Chemical Engineers (AIChE) Margaret Rousseau Pioneer Award. Karthish Manthiram received an MIT Teaching with Digital Technology Award and was named one of AIChE's 35 Under 35. Brad Olsen was named the new Kasser Professor. Greg Stephanopoulos was awarded an Advanced Research Projects Agency–Energy grant to decrease carbon emissions from biofuel production. Professor Emeritus Jeff Tester was elected to the National Academy of Engineering.

Despite the challenges of the Covid-19 pandemic, it was an exciting year of research for the department, with many new developments coming out of Chemical Engineering laboratories. Daniel Anderson's lab developed nanoparticles that can turn off genes in bone marrow cells. Martin Z. Bazant and colleagues developed a method to assess Covid-19 transmission risks in indoor settings. The related app and massive open online course (MOOC) expanded the reach of this research. Paul Barton received a grant from MITEI for technologies that avoid carbon emissions. Daniel Blankschtein turned his legendary thermodynamics lectures into a textbook. Arup Chakraborty (with Andrey Shaw) published a primer on viruses, vaccines, and therapies. Patrick Doyle developed a new platform for controlled delivery of key nanoscale drugs that may lead to smaller pills. T. Alan Hatton's lab developed a controllable membrane to pull carbon dioxide out of exhaust streams. Bob Langer and his team discovered how the surfaces of silicone breast implants affect the immune system. Startup Osmoses, spun out from the lab of Zachary Smith, won the MIT $100K Entrepreneurship Competition. Michael Strano's lab developed a new material made from carbon nanotubes that can generate electricity by scavenging energy from its environment. The lab also worked with colleagues to engineer a plant-based sensor to monitor arsenic levels in soil and helped in developing a heated face mask to filter and inactivate coronaviruses.

A more complete account of research conducted by and awards and recognition received by members of the department is given below.

Undergraduate Education

The Department of Chemical Engineering offers bachelor of science (SB) degrees in chemical engineering (Course 10) and chemical-biological engineering (Course 10-B) and a flexible SB degree in engineering (Course 10-ENG). The 10-ENG program leading to the engineering SB degree was introduced in response to demand from our students for a curriculum that would allow specialization in particular topics. The concentrations include biomedical, energy, environmental, materials process and design, society, engineering, ethics, computation, manufacturing design, and process data analytics. Thirty-three SB degrees were conferred in February and June 2021, 48% of which were awarded to women. The distribution of undergraduate students by class over the last 10 years is shown in Table 1.

Table 1. Undergraduate Enrollment

Class Year	2012	2013	2014	2015	2016	2017	2018	2019	2020	2021
Sophomores	72	61	67	57	56	58	44	41	42	36
Juniors	73	63	63	66	53	51	53	37	44	41
Seniors	75	69	58	64	67	55	50	59	42	42
Total	**220**	**196**	**188**	**187**	**176**	**164**	**147**	**137**	**128**	**119**

The department advises students about career paths in chemical and chemical-biological engineering through active participation in first-year advising seminars, fall and spring term open houses, Family Weekend, and other activities. In addition, the department has introduced several exploratory subjects for first-year students to learn about our major, as well as various outreach and extracurricular activities such as department-wide undergraduate project-lab presentations and prizes, ChemE Research Day, Science Slam, undergraduate chemical engineering career seminars, social events with faculty members, and the Bio-Maker Space (developed jointly with Biological Engineering), the first "wet" makerspace on campus.

AY2021 was unusual in that the campus was not easily accessible to undergraduate students due to restrictions placed on the Institute to protect the health and well-being of students, faculty, and staff. In response to the Covid-19 pandemic, the department's undergraduate courses were primarily offered remotely, with some lab-based courses offered in a hybrid format (remote lectures and in-person labs) based on students' expected graduation date and need to complete their lab requirements prior to the reopening of the campus. All seminars, open houses, presentations, lectures, and student group and recruitment events were hosted remotely. In addition to the remote offerings, the MIT Academic Policy and Regulations Team determined that a letter grading system with extra flexibility would be in effect for the year.

The senior survey indicates that 25% of our students are going on to graduate or professional school.

Undergraduates in the Department of Chemical Engineering maintain an active student chapter of the American Institute of Chemical Engineers, with invited speakers, presentations at national meetings, and visits to company sites. The chapter's student officers are Caroline Kenton, Kara Zhang, Danica Dong, Britney Pham, Daiyao Zhang, Ashleigh Teygong, Ming Yang, Nicole Munne, Ruoxin Lu, Julie Tung, Shuxin Chen, Sydney Vleck, Jacky Chin, Evan Gwozdz, Paula Pieper, Binette Wadda, Seraphine Castelino, Andison Tran, and Juan Aleman.

Graduate Education

The graduate program in the Department of Chemical Engineering offers master's of science degrees in chemical engineering (MS) and chemical engineering practice (MSCEP), doctor of philosophy (PhD) and doctor of science (ScD) degrees in chemical engineering, and the doctor of philosophy degree in chemical engineering practice (PhDCEP). The PhDCEP track was established in 2000 in collaboration with the Sloan School of Management.

The total graduate student enrollment is currently 224, with 213 in the doctoral program and 11 master's-level degree candidates. In the doctoral program, 204 students are in the PhD/ScD track and nine in the PhDCEP track. In the master's-level program, 11 students are in the MSCEP track. Thirty-five percent of our graduate students are women, and 4% are members of underrepresented minority groups. Forty-six of our graduate students were recipients of outside fellowship awards, including awards from the National Science Foundation (NSF), NIH, and the US Department of Defense (DOD). The distribution of graduate students by degree level over the last 10 years is shown in Table 2. During AY2021, 31 doctoral degrees (PhD, ScD, PhDCEP) and 20 master's-level degrees (MSCEP, MS) were awarded.

The department received 534 applications for admission to the doctoral program and offered admission to 55 individuals; 33 students accepted the offer (an acceptance rate of 60%). There were 117 applications for master's-level degrees; the department made 13 offers, 11 of which were accepted (a yield of 85%). Among the incoming graduate class, 14 students are women and five are members of underrepresented minority groups.

Table 2. Graduate Enrollment

Degree Level	2012	2013	2014	2015	2016	2017	2018	2019	2020	2021
Master's	20	10	11	15	15	10	12	13	14	11
Doctoral	224	212	211	222	218	222	214	224	197	213
Total	**244**	**222**	**222**	**237**	**233**	**232**	**226**	**237**	**211**	**224**

Research Centers

The Department of Chemical Engineering is actively involved and takes a leadership role in several Institute-wide education and research programs. A few of these programs are highlighted below. As faculty research officer, Professor Braatz facilitated the continuous updating and evolution of the department's strategic plan and the generation of multiple-faculty proposals to support the specific research directions defined in the plan.

Data-Driven Design of Li-ion Batteries

The Toyota Research Institute renewed Professors Bazant and Braatz's Data-Driven Design of Li-ion Batteries (D3BATT) joint center for another four-year period. D3BATT is developing a multiscale modeling framework for rechargeable batteries to accelerate materials discovery and design. This year's publications included an invited perspective on combining physics and machine learning to predict battery lifetime and a paper in *Nature Materials* showing that heterogeneous delithiation in layered oxide cathodes, which had been attributed in the literature to phase separation, is actually the result of autocatalytic reactions.

Smart Data Analytics in Biomanufacturing

Professors Braatz, Anthony Sinskey (Biology), and Retsef Levi (Sloan) and Stacy Springs (Center for Biomedical Innovation) co-lead the Smart Data Analytics for Risk Based Regulatory Science and Bioprocessing Decisions project, which is funded by the US Food and Drug Administration (FDA). Open-source software packages have been released that (1) automate optimal selection of machine learning algorithms for biopharmaceutical manufacturing applications to generate solutions at the same level of performance as a team of experienced human experts and (2) are able to learn first-principles relationships that arise in physical, chemical, and biological systems.

Accelerated Molecular Discovery Project

Professor Klavs Jensen continued to lead the Defense Advanced Research Projects Agency Accelerated Molecular Discovery project, which aims to accelerate the pace of chemical innovation through data extraction by developing new predictive models based on a combination of literature data, physical knowledge, and new high-throughput experiments. In collaboration with Professors Regina Barzilay and Tommi Jaakkola from Computer Science and Professor Green, the team combined machine learning property prediction and generative models with a new automated, high-throughput experimental platform to realize autonomous molecular discovery. The experimental program was delayed during the campus shutdown but is back on schedule. The team used the remote working environment to advance database, automation, and machine learning algorithms.

Machine Learning for Pharmaceutical Discovery and Synthesis Consortium

Professors Barzilay, Green, Jaakkola, and Jensen continued to work with members of the MIT-industry Machine Learning for Pharmaceutical Discovery and Synthesis Consortium (MLPDS) (Amgen, AstraZeneca, BASF, Bayer, Bristol Myers Squibb, GSK, Janssen, Leo Pharm, Lilly, Merck, Novartis, Pfizer, Sunovion, Syngenta, and WuXi). The consortium brings together scientists and engineers from member companies and MIT to create new data science and artificial intelligence (AI) algorithms along with tools to facilitate the discovery and synthesis of new therapeutics. MLPDS educates scientists and engineers to work effectively at the data science/chemistry interface and provides opportunities for member companies and MIT to collectively create, discuss, and evaluate new advances in data science for chemical and pharmaceutical discovery, development, and manufacturing. Company and MIT researchers continued to meet and collaborate during the pandemic through multiple online platforms.

Disruptive and Sustainable Technology for Agricultural Precision

The Disruptive and Sustainable Technology for Agricultural Precision (DiSTAP) Interdisciplinary Research Group, part of the Singapore-MIT Alliance for Research and Technology (SMART), completed a highly successful third year in partnership with the Temasek Life Sciences Laboratory in Singapore. Since its kickoff in 2018, the $40 million initiative has been producing next-generation sensors and analytical instrumentation, plant delivery, and environmental tools for the urban farm of the future. The DiSTAP team, led by Professor Strano, welcomed Associate Professor Benedetto Marelli (Course 1) as a full member this year. Professor Marelli's pioneering work on silk-based technology will accelerate advances in seed technology, food packaging, and sensor interfaces for precision agriculture. This year, DiSTAP principal investigator (PI) Rajeev Ram (Course 6) showcased powerful and field-portable sensor technology that allows for Raman spectroscopy and nanosensor signals to be gathered at considerable distances from crops to monitor key indicators. The DiSTAP group published an invited perspective article in the journal *Nature Plants* on technology to shape the future of agriculture.

Center for Enhanced Nanofluidic Transport

The Center for Enhanced Nanofluidic Transport (CENT), an $11 million Energy Frontier Research Center funded by the US Department of Energy, completed a successful third year. The center is led by Professor Strano, its founder and scientific director, as well as other Course 10 faculty. CENT is focused on what we identify as knowledge gaps in our basic understanding of fluidic transport under extreme confinement. The center is producing fundamental insights into geologic transport and new membrane and other separation technologies for energy efficiency. This year CENT made pioneering advances in understanding ion solvation, nanofluidic transport, and membrane technology. In one highlight, Strano and his team took the bold step of turning the original CENT proposal into a review article documenting emerging knowledge gaps in the nanofluidics field. The article is now listed as a "Highly Cited Paper" by Web of Science due to its rate of citation, underlining the significant intellectual impact being made by the center. The CENT PIs mourned the loss of one of the center's original founders, Professor Mark Reed of Yale, who died suddenly at his home in May 2021, and remain committed to honoring Mark's legacy.

Faculty Notes

Robert Armstrong is the director of the MIT Energy Initiative. MITEI continues to grow rapidly in its research, educational, and outreach components. Ten companies sponsor research as founding, sustaining, and startup members of MITEI. Altogether, the energy initiative is engaged with more than 80 industrial and public partners and individual members across five continents. MITEI has helped to bring in approximately $850 million in support during the past 10 years of its operation, along with 400 energy fellowships spread over 25 departments. The MITEI Low Carbon Energy Centers (LCECs), announced in 2015 as key components of MIT's Climate Action Plan, continue to develop. We recently announced the new Future Energy Systems Center as part of MIT's Climate Action Plan for the Decade. This center leverages the capabilities of the LCECs to understand how the energy system can evolve regionally and globally to achieve ambitious net-zero emissions targets. Professor Armstrong serves on the scientific commission of the Eni Enrico Matteo Foundation, the editorial board of *World Energy* magazine, the external scientific advisory committee of Argonne National Laboratory, and the board of directors of the National Renewal Energy Laboratory. In addition, he serves on the advisory boards of numerous academic programs.

Daniel Blankschtein's group carries out modeling/simulation and experimental research in the area of colloid and interface science, with an emphasis on practical applications. He interacts with several companies that make use of software developed by his group to facilitate surfactant formulation design. The group presented invited talks, regular talks, seminars, and posters at various scientific meetings in the United States and abroad. Professor Blankschtein is a member of the DOE Center for Nanofluidic Transport (CENT). In the context of CENT, his group is investigating the thermodynamic and transport behavior of fluids, particularly water and aqueous electrolytes, under extreme confinement, including developing novel polarizable force fields to model relevant interactions at the nanoscale. In addition, Professor Blankschtein's group is investigating, both theoretically and experimentally, nanoporous graphene membranes for gas separation. Blankschtein continues to serve on the editorial board of Marcel

Dekker's Surfactant Science Series. In March 2021, his new book titled *Lectures in Classical Thermodynamics with an Introduction to Statistical Mechanics* was published by Springer.

Richard D. Braatz continued research in applied mathematics and control theory and its application to chemical and biological systems. He led the systems research in many advanced manufacturing projects, including research with approximately $9 million of support from the US Department of Health and Human Services to validate methodologies in fully automated experimental platforms for biopharmaceutical manufacturing. Results from his group include the first mechanistic model for the commercially important triple transfection process used in gene therapy manufacturing based on recombinant adeno-associated viruses and open-source software for advanced process control and data analytics and machine learning. He gave many plenaries and keynote lectures, including talks on mechanistic modeling, control, and data analytics for advanced biopharmaceutical manufacturing systems. He served on the scientific advisory boards for a biotechnology company and a NASA Science and Technology Research Institute that is developing biological and energy technologies for the survival of humans in outer space, and he is a member of the board of trustees for a nonprofit corporation that develops computing tools for chemical engineering education. He served as past president of the American Automatic Control Council, a federation of nine professional societies that organizes the largest annual control conference in the United States.

Fikile R. Brushett, Cecil and Ida Green Career Development Chair and Associate Professor of Chemical Engineering, leads a research group that focuses on advancing the science and engineering of electrochemical systems needed for a sustainable energy economy. This past year, his group's original research contributions included the synthesis and characterization of porous electrode materials for redox flow batteries and the computational modeling of electrochemical reactors. Professor Brushett was recognized with the National Organization for the Professional Advancement of Black Chemists and Chemical Engineers NOBCChE Lloyd N. Ferguson Young Scientist Award for Excellence in Research as well as the NESACS-NOBCChE Henry Hill Keynote Lecture. At MIT, he served on several department and institute-wide committees including the Committee on the Undergraduate Program and RIC-7: Career Support for Postdocs, Research Scientists, and Instructional Staff. He also continued to serve as a freshman advisor and as a contributor to the upcoming MIT Energy Initiative Future of Storage study. Outside MIT, Professor Brushett continued in his role as the research integration co-lead for the Joint Center for Energy Storage Research (JCESR), a DoE funded energy innovation hub.

Arup K. Chakraborty continued 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 also an important facet. Chakraborty, in collaboration with Professors Phillip Sharp and Laurence Young, also continued to work on a project initiated in 2016 on understanding how genes critical for maintaining healthy cell states are regulated. Chakraborty researched Covid-19 in AY2021, and his HIV work has led to an immunogenic vaccine in monkeys, with efforts under way to move the concept to humans. Chakraborty published a general audience book, *Viruses, Pandemics,*

& Immunity, that has been well received. In 2020, Chakraborty was presented the Outstanding Graduate Faculty Award for his classroom teaching based on student votes, and he received AIChE's Prausnitz Institute Lectureship Award. Also, he was appointed an Institute Professor and a member of the board of governors of the Wellcome Trust.

Kwanghun Chung continued to lead an interdisciplinary research team that develops and applies novel technologies for a holistic understanding of large-scale complex biological systems. Recent research advances by the Chung lab include the development of ELAST technology that transforms human brain tissues into elastic hydrogels to enhance macromolecular accessibility and mechanical stability simultaneously and the creation of SCOUT technology that enables high dimensional phenotyping of organoid disease models. He led several large multi-PI projects, including a $9 million NIH human brain mapping project and a $5 million NIH reusable antibody development project, to apply his technologies for mapping and studying the human brain. In addition, his group has active collaborations with many researchers at MIT, the Broad Institute, Massachusetts General Hospital, and Harvard to study various neurological disorders such as autism spectrum disorder and Alzheimer's disease. Over the past year, Professor Chung taught 10.302 Transport Processes and HST.562 Pioneering Technologies in Biology and Medicine. He also served on the Institute for Medical Engineering and Science (IMES) Committee for Academic Programs and the department's graduate admission committee. In addition, he continued serving as a chief scientist for LifeCanvas Technologies, a startup that aims to advance the adoption and usage of three-dimensional tissue molecular phenotyping technologies.

Connor W. Coley, the Henri Slezynger (1957) Career Development Chair, started as an assistant professor in the Department of Chemical Engineering in 2020. He leads an interdisciplinary group of students seeking to expand the role of computer assistance and automation in the design and synthesis of small molecules, with an eye toward the autonomous discovery of small molecule therapeutic candidates. The Coley group's research focuses on the development and application of new machine learning methods tailored to the domain of chemistry. The lab is currently supported by MLPDS, the MIT-IBM Watson AI Lab, J-Clinic, Takeda, Nanite Bio, the Office of Naval Research, and the Royal Society of Chemistry. He has given 27 invited talks since July 2020 and has published several articles in journals such as *Chemical Science* and the *Journal of Chemical Information and Modeling*. Professor Coley taught the 10.34 Numerical Methods and 10.551 Systems Engineering graduate courses in AY2021 and co-created the new 10.402/10.602 Machine Learning for Molecular Engineering elective course. He serves on the advisory boards of three startup companies and one NSF center.

Charles L. Cooney, Robert T. Haslam (1911) Professor of Chemical and Biochemical Engineering, emeritus, taught 10.491 Integrated Chemical Engineering, which introduces chemical engineering seniors to batch processes through the design of a manufacturing facility for therapeutic monoclonal antibodies. He also teaches 10.547 Principles and Practice of Drug Development. Professor Cooney continues as an advisor to the SMART Innovation Center in Singapore and as a member of the steering committee of the Deshpande Center for Technological Innovation. He is the faculty director of the Downstream Processing summer course held through MIT's Professional Institute.

Professor Cooney is a member of the board and executive committee of the Norman B. Leventhal Map and Education Center at the Boston Public Library, an advisor emeritus of the Boston Symphony Orchestra, a trustee emeritus of the Boston Ballet, and a member of the advisory boards of the National Institute for Bioprocessing Research and Training in Ireland, the Biopharmaceutical Analysis Training Laboratory at Northeastern University, and the Gloucester Marine Genomics Institute.

Patrick S. Doyle, Robert T. Haslam (1911) Professor of Chemical Engineering, continues to serve as the graduate officer for the department. His research focuses on soft matter, including fundamental studies of DNA polymer physics, miRNA sensing, and microfluidic synthesis of functional microparticles. He was honored with an appointment as a Singapore Research Professor Chair in 2020. His research on new ways to remove micropollutants from water won the Judges Choice Award for Potential Scalability at the J-WAFS World Water Day video competition. He continues to lead two major efforts in Singapore (funded through CREATE and the Pharma Innovation Programme Singapore) focusing on new methods for formulating small molecule drugs. In a significant study published in *Advanced Material Technologies*, his group developed a continuously embedded droplet printing method in yield-stress fluids for pharmaceutical drug particle synthesis. Professor Doyle delivered several invited lectures at company meetings, conferences, and universities, including Swiss Soft Matter Days. He currently serves on the scientific advisory boards of Withings and Achira Labs and is a member of the visiting committee of the National University of Singapore Chemical Engineering Department.

Ariel Furst, the Raymond (1921) & Helen St. Laurent Career Development Professor of Chemical Engineering, leads a research group that combines electrochemistry with biochemical engineering to improve human and environmental health. The current group members (three graduate students, two postdocs, and nine undergraduate students) are working on electrochemical strategies to detect and combat antibiotic resistance in bacteria, diagnose Covid-19, detect and degrade environmental contaminants, and upcycle carbon dioxide. Research in the group is currently supported by MITEI, J-WAFS, NIH, the Deshpande Center, and RSC. Professor Furst published 10 papers during the past year and was invited to give presentations at the American Chemical Society (ACS) Sensors Young Investigator Symposium and the Electrochemical Society Dennis Peters Retrospective Symposium. She is working to increase active learning and practical skills in courses by developing the graduate-level 10.594 Bioelectrochemistry Course and revamping the 5.310 Chemistry Laboratory course for non-majors. She is a member of the Chemical Engineering DEI Committee and has founded DEI book clubs for undergraduates and incoming graduate students.

Katie Galloway, a chemical engineer working in molecular systems biology, joined the department in July 2019. Her group focuses on elucidating the fundamental principles of integrating synthetic circuitry to drive cellular behaviors. Her research has been featured in *Science* and *Cell Stem Cell*. She is the recipient of the NIH Ruth L. Kirschstein National Research Service Award Postdoctoral Fellowship and the California Institute of Technology's Everhart Award. Her group constructs genetic controllers capable of dynamically routing cells toward diverse fates. The lab has pioneered key methods for building and validating RNA- and DNA-based regulatory elements and controllers and developed foundational technologies for engineering highly efficient cellular reprogramming to neurons. In the last year, the group's work has been published in *Cell Systems*, *Current Opinion in Systems Biology*, and *Nature Reviews Molecular Cell Biology*. As an instructor for 10.10 Introduction to Chemical Engineering, Professor Galloway continues to develop new methods of engaging students. In 2020, she developed two training programs in computational modeling and digital research methods for undergraduate researchers performing remote Undergraduate Research Opportunities Program projects.

William H. Green and his students developed a model for predicting solvation energies that is more accurate than most experimental measurements, invented an efficient way to include quantum-mechanical information in machine learning models based on experimental data, published a new version of the Reaction Mechanism Generator software package, and discovered why the ignition of ethers has such peculiar dependence on pressure. His perspective on the ongoing transition from postdictive to predictive kinetics was featured on the cover of the *AIChE Journal*. He continues to serve as co-chair of MITEI's Mobility Systems Center and MIT's Climate Grand Challenge effort on hard-to-decarbonize transport sectors (long-distance aviation, shipping, and trucking).

This year Paula Hammond was appointed to an Institute Professorship, considered the highest honor given to an MIT faculty member. She also became a Hagler Fellow at Texas A&M University and delivered the J.C. Smith Lecture at Cornell University, the Schwarz Lecture at Johns Hopkins University, and the Pioneers Lecture at the University of Toronto. Her research program continues to focus on nanoparticle delivery systems to address ovarian cancer and glioblastoma as well as materials for cartilage regeneration to treat osteoarthritis and scaffolds for bone repair. Along with serving as the department head, she is the faculty co-chair of the Ad Hoc Committee on Graduate Advising and Mentoring.

As noted, T. Alan Hatton continued to serve as the director of the David H. Koch School of Chemical Engineering Practice; during Covid-19, his student teams successfully worked remotely with host companies Corning, Astra-Zeneca, Merck, and Schlumberger. A new course was floated during Independent Activities Period (IAP)—10.801 Project Management and Problem Solving on Academia and Industry—to better prepare Practice School students for professional careers. Professor Hatton is a co-director of the MITEI Low Carbon Energy Center on Carbon Capture, Utilization and Storage, and in this role he participated in a number of MITEI workshops and meetings. Over the past year, he delivered invited keynote and plenary lectures remotely at national and international meetings as well as universities. Hatton continues to develop new directions for mitigation of environmental problems, primarily electrochemical approaches to carbon capture and micro-contaminant removal from aqueous sources.

Klavs F. Jensen's lab continued its efforts in collaboration with Eli Lilly and Pfizer to use automated platforms to explore chemical transformations, optimize chemical reactions, and extract chemical kinetics. Also, Professor Jensen worked with Professor Olsen to extend these automated synthesis and machine learning approaches to polymer synthesis. Professor Jensen continued to co-direct (with Professor Barzilay) the MIT-industry Machine Learning for Pharmaceutical Discovery and Synthesis Consortium.

During the past academic year, he devoted considerable effort to teaching his 10.492B Integrated Chemical Engineering and 10.65 Chemical Reactor Engineering classes online. Working remotely, he continued to deliver lectures at international conferences, publish in leading journals, and serve on scientific advisory and editorial boards.

Professor Jesse H. Kroll and his research group continued their work on the organic chemistry of the atmosphere, the formation and evolution of atmospheric particulate matter, and air quality measurements using low-cost sensors. Group publications included work on the atmospheric chemistry of inorganic and organic nitrates, deployment of a low-cost sensor network in Hawaiʻi to measure volcanic pollution during the 2018 Kīlauea eruption, and the role of Covid-19-related shutdowns in air quality and atmospheric chemistry. A new research focus has been the atmospheric chemistry of indoor environments. Professor Kroll is director of the R. M. Parsons Laboratory for Environmental Science and Engineering and serves on the board of directors of the American Association for Aerosol Research.

Heather J. Kulik leads a group that carries out interdisciplinary research in computational first-principles modeling and machine learning for accelerated inorganic design and large-scale, predictive modeling of catalyst (both biological and nonbiological) and materials properties. Major accomplishments in the past year included models for predicting the stability of new metal-organic framework (MOF) materials and new consensus-based approaches to materials discovery. This past year, Professor Kulik received an Alfred P. Sloan Fellowship in Chemistry and a Molecular Systems Design & Engineering Outstanding Early-Career Paper Award. She presented more than 20 virtual invited talks and keynotes at both national and international conferences and universities and published over 15 peer-reviewed papers, including profiled articles in *ACS Central Science* and *Chemical Science*. In addition to collaborations with industry, her group's research is supported by the DOD, DOE, and NSF. Kulik teaches the undergraduate 10.37 Chemical Kinetics and Reactor Design course and continues to develop her 10.637 Quantum Chemical Simulation elective, which provides an immersive experience in simulation and has been well received both across the Institute and by neighboring institutions. The Kulik group consists of five postdocs, 12 graduate students, and several visiting and undergraduate researchers.

In 2020, Institute Professor Robert Langer published 32 papers and delivered numerous lectures. In addition, he served on seven Institute boards and a number of industry boards. Professor Langer is a consultant to the US State Department, the National Academy of Sciences, the National Academy of Engineering, the National Academy of Inventors, the National Academy of Medicine, and the FDA. His efforts were recognized with the Medalha da Ciência (the Portuguese government's highest distinction for scientists), the Maurice-Marie Janot Award, and the Surfaces in Biomaterials Foundation's Excellence in Biomaterials Science Award. He was elected a fellow of the American Association for Cancer in 2020.

J. Christopher Love, Raymond A. (1921) and Helen E. St. Laurent Professor of Chemical Engineering, led a research team that contributed to the advancement of clinical-stage vaccine candidates for Covid-19 intended for low-cost, global access. The lab contributed new designs of protein subunits with enhanced immunogenicity and strains engineered to produce them at industrial facilities. In collaboration with the Gates Foundation and others, the lab demonstrated the efficacy of one candidate in non-clinical studies and is developing new candidates based on the evolving variants of SARS-CoV-2. In addition to this contribution to the global pandemic response, Professor Love continued to lead an MIT-industry consortium directed at the advancement of alternative hosts for biopharmaceuticals and vaccines (AltHost). This collaborative, open-source approach founded at MIT is creating engineered strains for efficient and high-quality proteins with an aim toward lowering the costs and time lines for development of manufacturing approaches. He and his lab also continued to advance understanding of food allergies and related disease-like eosinophilic esophagitis using their unique nanowell-based approach for single-cell RNA sequencing developed with Professor Alex Shalek (Chemistry/IMES) and his lab. He continued to serve as a scientific advisor to several companies, including startups commercializing technologies developed in the lab.

Karthish Manthiram is an assistant professor of chemical engineering and holds the Theodore T. Miller Career Development Chair. He leads a research group that develops methods by which carbon dioxide, nitrogen, and water can be converted into diverse chemicals using renewable electricity. In 2021, Professor Manthiram was awarded a Sloan Research Fellowship. He continues to be involved in activities designed to shape policy and research in the United States, including an invited talk he gave to the National Academies of Science, Engineering, and Medicine, which has convened the Committee on Enhancing the U.S. Chemical Economy through Investments in Fundamental Research in the Chemical Sciences. He is serving as a member of the faculty steering committee of the newly formed MIT Climate and Sustainability Consortium, on which he has been focused on developing a new postdoctoral fellowship program. His group has made key advances in the last year, including developing new Bayesian statistics analysis methods for robust analysis of electrochemical kinetic data and methods by which energy sources that drive chemical reactions can be distinguished on a thermodynamic basis Professor Manthiram was presented the Camille Dreyfus Teacher-Scholar Award, which recognizes excellence in both teaching and research in the chemical sciences.

Allan S. Myerson continued his research on fundamental and applied problems in crystallization and pharmaceutical manufacturing. He is a principal investigator on projects related to use of image analysis and machine learning for the control of pharmaceutical unit operations, continuous manufacturing of a pharmaceutical intermediate, and novel crystallization methods using plug flow crystallizers. He serves as a scientific advisor to Circ, CONTINUUS Pharmaceuticals, and On Demand Pharmaceuticals, companies that are commercializing various aspects of continuous pharmaceutical manufacturing.

Bradley D. Olsen, the Alexander and I. Michael (1964) Kasser Professor of Chemical Engineering, was recognized this year with the ACS Macromolecules/Biomacromolecules Young Investigator Lectureship. Olsen's research group continued its work in the areas of polymer sustainability, biopolymers, and polymer networks, with the group also leading a major new database initiative in the area of big data and new informatics tools for polymers. This Community Resource for Innovation in Polymer Technology aims to provide a community resource for the development of new polymer materials and sustainable solutions to materials challenges, enabling faster sharing, search, and analysis of data. Other major accomplishments of the group included new theories for gel fracture and swelling and the development of new processes for rubber recycling. The group published 14 papers. Professor Olsen served as an instructor for 10.40 Chemical Engineering Thermodynamics, a core graduate class, and 10.00 Molecule Builders, a lab experience for first-year students and sophomores in molecular design. He was also faculty director of the MISTI Brazil program, chair of Chemical Engineering admissions, and a member of the steering committee assembled to found a new department of biomedical engineering at the Hospital Albert Einstein in São Paulo, Brazil.

Kristala L. J. Prather, the Arthur D. Little Professor of Chemical Engineering and a member of the Synthetic Biology Center, continues to focus on microbial synthesis of chemical compounds. Her most recent service to the profession includes appointments to the National Academies Committee on Enhancing the U.S. Chemical Economy and to the World Economic Forum Global Future Council on Synthetic Biology. Prather also assumed the presidency of the International Metabolic Engineering Society. She became a fellow of the American Institute of Chemical Engineers and will be recognized as the recipient of the Andreas Acrivos Award for Professional Progress in Chemical Engineering at the next AIChE annual meeting. Prather continues to serve as director of the MIT Professional Education Fermentation Technology short course along with other continuing leadership roles. She was appointed co-chair, with Professor Tyler Jacks (Biology/Koch Institute), of the Vision to Integrate, Translate and Advance Life Committee on Life Sciences and Engineering. This spring she was honored as a recipient of the Gordon Y. Billard Award at the Institute Awards Convocation.

Gregory C. Rutledge and his research group study fundamental relationships in processing and crystallization of macromolecules, fiber-forming polymers, and applications of polymeric nanofibers. Over the past year, they continued their development of a multiscale model of flow-induced crystallization, heterogeneous nucleation, composites, and separations using nanofiber membranes. In response to Covid-19, Professor Rutledge served on the Massachusetts Manufacturing Emergency Response Team and his group developed alternative personal protective equipment materials; this work has been highlighted in Project Frontline. Rutledge is the lead PI for MIT at Advanced Functional Fabrics of America and heads up a team of researchers from the School of Science, the School of Engineering, and the Sloan School of Management that is responding to MIT's Climate Grand Challenge with a plan for emissions reduction through innovation in the textile industry. On the educational front, Rutledge was in charge of the in-person 10.26/27/29 Chemical Engineering Projects Lab during the Covid-19 restrictions on campus and the collaborative MIT-FIT Workshop on Advanced Fibers and Fabrics. He also serves as editor of the *Journal of Materials Science*.

Zachary P. Smith is an assistant professor of chemical engineering. In the past year, he was awarded the Institute-wide Robert N. Noyce Career Development Chair and received the ONR Young Investigator Award and the AIChE 35 Under 35 Award. He published nine peer-reviewed papers, including papers in *Chemical Reviews*, *Angewandte*

Chemie, *ACS Nano*, *Macromolecules*, and *Polymer*, and presented five invited talks. Professor Smith serves on the board of directors of the North American Membrane Society and the editorial advisory board of *Polymer*. He filed two patent applications this year and cofounded a startup company, Osmoses Inc., to translate developments from his lab into commercial membrane modules. Professor Smith taught 10.467 Polymer Science Lab in the fall and 10.32 Separations in the spring. He was presented the MIT Frank E. Perkins Award for Excellence in Graduate Advising. He supervises five postdoctoral scholars/fellows, 10 graduate students, and four undergraduate researchers. He graduated his first two PhD students this year and sent two postdoctoral scholars to positions in academia (Nankai University and Hunan University in China).

Gregory Stephanopoulos, the W.H. Dow Professor of Biotechnology and Chemical Engineering and director of the Metabolic Engineering Laboratory, continued research on microbe engineering for natural product biosynthesis and production of fuels and chemicals via biological non-photosynthetic CO2 fixation. Notable advances included strain construction for the production of carotenoids and other products from acid whey, the waste stream of Greek yogurt manufacturing, advancement of CRISPR technologies for efficient editing of oleaginous yeasts, and engineering of oleaginous yeasts for alkane production. His group also reported engineering of yeast for enhanced tolerance to toxic compounds, leading to dramatic increases in ethanol production from cellulosic biomass. These technologies bring us closer to the vision of a biobased economy. To support this work, four new grants from NSF and DOE were obtained. Professor Stephanopoulos continued on the advisory boards of four academic institutions and the managing board of the Society for Biological Engineering. He serves as editor-in-chief of *Current Opinion in Biotechnology* and on the editorial boards of eight other scientific journals. Due to Covid-19, his research presentations at meetings were replaced by numerous virtual presentations. Professor Stephanopoulos received the honor of having the Metabolic Engineering Award named after him.

Carbon P. Dubbs Professor Michael S. Strano continued research at the interface of nanotechnology and chemical engineering. Over the past year, his laboratory published a new discovery of electrochemical energy generation at a particle from the surrounding solvent. The asymmetric chemical doping mechanism was published in *Nature Communications* and promises wireless electrocatalysis and self-powered micro-robots. The group also published (in *Nature Plants*) a nanosensor for living plants that intercepts and communicates the plants' internal stress waves. Such nanosensors allow the detection of chemical waveforms for specific types of stress. Strano and his team are busy using reaction and diffusion models to decode these waveforms. They were also busy throughout the pandemic developing a new virucidal mask using chemical engineering principles. Professor Strano continues as lead PI of DiSTAP, which this year showcased new sensor technology for precision agriculture. He also continued as scientific director of the Center for Enhanced Nanofluidic Transport.

James Swan's group performs fundamental theoretical research in the areas of soft matter physics and fluid mechanics. Recent work has focused on developing new simulation methods capable of modeling complex soft materials at the meso scale and applying those methods to materials of industrial and societal interest, including food and consumer care products and biopharmaceuticals. Swan was promoted to associate professor with tenure in 2021. His group's work over the past year appeared in 15 peer-reviewed publications. A new research direction from his group focused on bringing machine learning and high throughput data acquisition to the field of rheology, spawning an industrial collaboration yielding several academic articles and new invention disclosures. The Swan group has produced seven PhDs over the last eight years and currently includes seven graduate students and a postdoc.

William A. Tisdale is a MacVicar Faculty Fellow and associate professor of chemical engineering. His research is dedicated to the development of novel solution-processable semiconductor nanomaterials for use in next-generation energy technologies. His research accomplishments have been recognized through numerous awards, including the Presidential Early Career Award in Science and Engineering and the DOE's Early Career Award. In the past year, Professor Tisdale delivered plenary lectures at the AIChE annual meeting and the first Internet Conference on Quantum Dots. He also served as general organizer for the nanoGe Spring Meeting, a European conference focused on nanomaterials in energy applications. Professor Tisdale is a faculty lead for the New Engineering Education Transformation Renewable Energy Machines Thread, serves as Course 10 representative at Institute faculty meetings, and is a faculty advisor to the student-led Baker Foundation Advisory Committee.

Professor Bernhardt L. Trout developed and continues to teach (with colleagues) the seminal 10.01 Ethics for Engineers course, which educates close to 15% of the MIT student body on ethical issues related to engineering. The course enhances the breadth and depth of engineering students' knowledge, teaching them the connections between engineering and society, and is a model for educating engineering students at MIT and around the world. Professor Trout's laboratory focuses on pharmaceutical small molecule manufacturing and biopharmaceutical formulation and stabilization, including predictive methods used by pharmaceutical companies around the world, as well as advanced manufacturing processes. He works closely with the FDA and other national regulatory authorities in addition to pharmaceutical manufacturing entities. In addition, he is on the scientific advisory boards of a number of major companies and involved in several startups. Over the past year, Professor Trout delivered many invited talks along with publishing research papers and submitting patents.

Research Highlights

Learning Battery Physics from Images (Martin Z. Bazant)

Traditional methods of scientific inquiry and engineering design begin with human intelligence: mathematical models encoding physical hypotheses are proposed, tested against experimental data, and refined by fitting adjustable parameters. Recent advances in artificial intelligence appear to challenge this paradigm, since predictions can be made directly from data without the need for models, but such knowledge is often not transferrable to new situations. Professor Bazant's vision for advancing science in this new era is to leverage large data sets to learn new physics as defined by unknown functions in general mathematical models, effectively combining human and machine learning.

In order to achieve this vision in the important engineering context of Li-ion batteries for electric vehicles, Professor Bazant founded the D3BATT center in 2017. D3BATT leverages experimental and modeling capabilities at MIT (including those of co-PI Richard Braatz) and Stanford that span length scales from microns to meters to learn the physics of batteries from large data sets of images (optical, X-ray, electon) and spectra (X-ray diffraction, acoustic emissions, electrochemical impedance) and develop physics-informed AI for battery performance optimization and prediction.

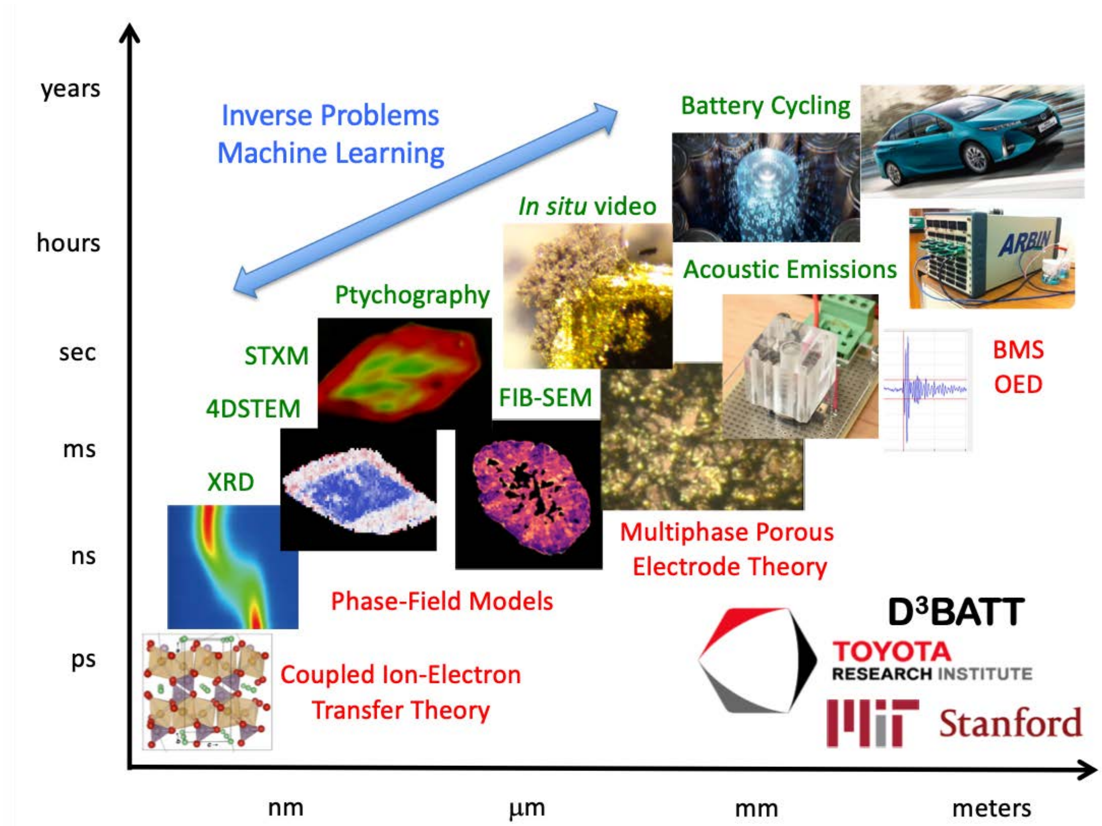
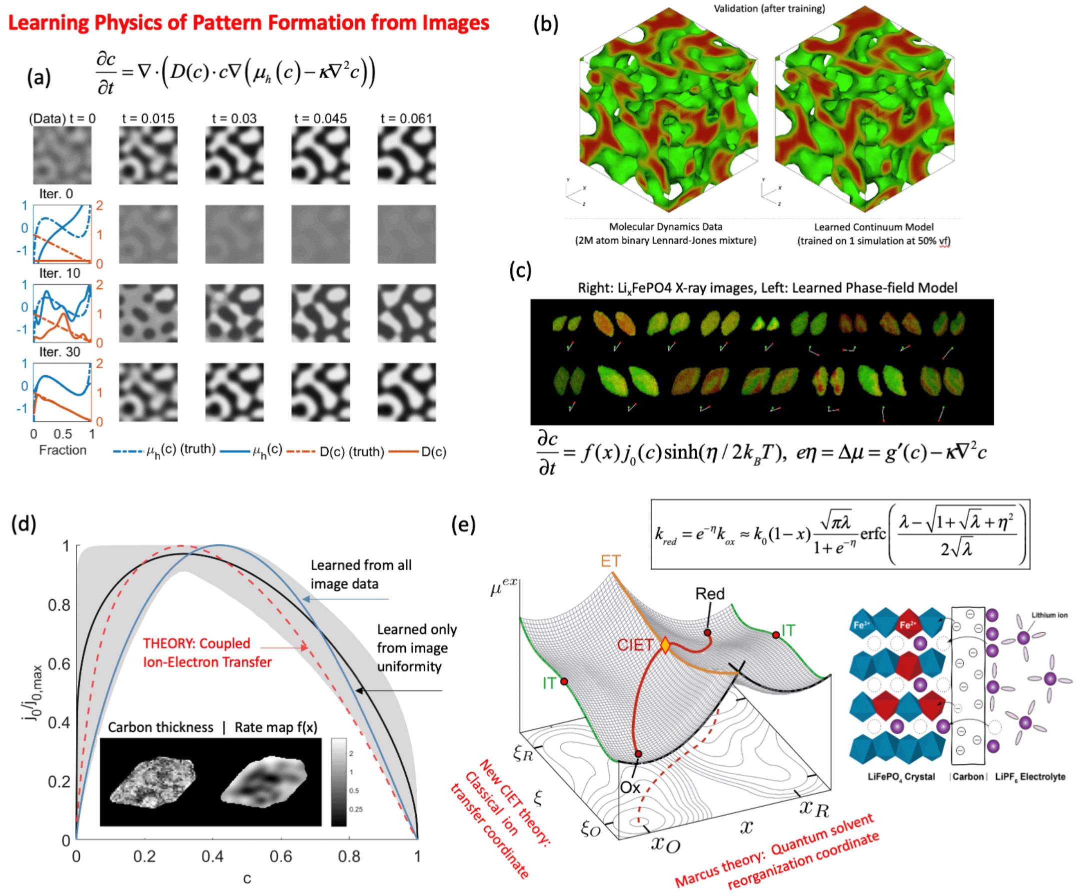


Figure 1. Multiscale data and models for physics-based AI to predict Li-ion battery performance and lifetime.

For example, we have recently developed a computational method of solving partial differential equation–constrained inverse problems to derive predictive, transferrable models of electrochemical nonequilibrium thermodynamics directly from image data. Examples include inferring electro-autocatalytic reaction models from X-ray diffraction spectra for nickel-rich metal oxide cathodes, optical videos of lithium metal growth on graphite anodes, and X-ray adsorption imaging of driven phase separation in lithium iron phosphate high-rate cathodes.



$$\frac{\partial c}{\partial t} = \nabla \cdot \left(D(c) \cdot c \nabla \left(\mu_h(c) - \kappa \nabla^2 c \right) \right)$$

$$\frac{\partial c}{\partial t} = f(x) j_0(c) \sinh(\eta / 2k_B T), \quad e\eta = \Delta\mu = g'(c) - \kappa \nabla^2 c$$

$$k_{red} = e^{-\eta} k_{ox} \approx k_0 (1-x) \frac{\sqrt{\pi\lambda}}{1+e^{-\eta}} \operatorname{erfc}\left(\frac{\lambda - \sqrt{1+\sqrt{\lambda}+\eta^2}}{2\sqrt{\lambda}} \right)$$

Figure 2. Learning physics from images. (a) Iterations of image inversion (bottom three rows) to learn approximations (solid lines) of the true unknown (dashed lines) concentration-dependent diffusivity (orange) and homogeneous chemical potential (blue) leading to solutions of the Cahn-Hilliard equation that reproduce a small set of simulated images (top row). (b) Applying the same method to learn a continuum phase-field model (right) that accurately reproduces molecular dynamics simulations (left) of spinodal decomposition. (c) Learning the reaction rate constant for lithium ion intercalation versus concentration and position on the surface in an Allen-Cahn reaction model from scanning transmission x-ray microscopy (STXM) images of lithium iron phosphate platelet nanoparticles (STXM image data on the left, learned simulation on the right). (d) The learned exchange current versus concentration from the image inversion agrees well with (e) the quantum-mechanical theory of coupled ion-electron transfer. Also shown in the inset of (d) is the inferred spatial variation of the reaction rate prefactor over a particle surface (right), which correlates well with independent measurements of the carbon coating thickness on the surface (left). This may be the first time that nanoscale spatial heterogeneity in surface coatings governing electrocatalytic reaction rates has been detected non-destructively over an electrode surface.

Covid-19 Indoor Safety Guideline (Martin Z. Bazant)

When the Covid-19 pandemic erupted in spring 2020, Professor Bazant became concerned that various safety protocols promoted by public health authorities, such as the Centers for Disease Control and Prevention's "six-foot rule" of social distancing, were not based on scientific analysis and yet were causing significant economic, educational, and social impacts for the young and healthy while risking deadly longer-range airborne transmissions among the elderly. For example, MIT was imposing strict six-foot distancing in highly ventilated labs designed to handle airborne toxins, while nursing homes in New York City were ordered to place Covid-positive patients in poorly ventilated shared rooms as long as the beds were six feet apart. By May 2020, Professor Bazant felt the need to take action and set out to study Covid-19 transmission and derive a physics-based safety guideline. By then, evidence was mounting (although largely ignored by public health authorities) that Covid-19 transmission was primarily airborne, via prolonged breathing of exhaled aerosol droplets, analogous to secondhand smoke. Bazant reached out to his colleague John Bush (Mathematics), who had studied the fluid mechanics of coughs, and they derived the first simple, quantitative safety guideline for airborne transmission and published a comprehensive article explaining the science.

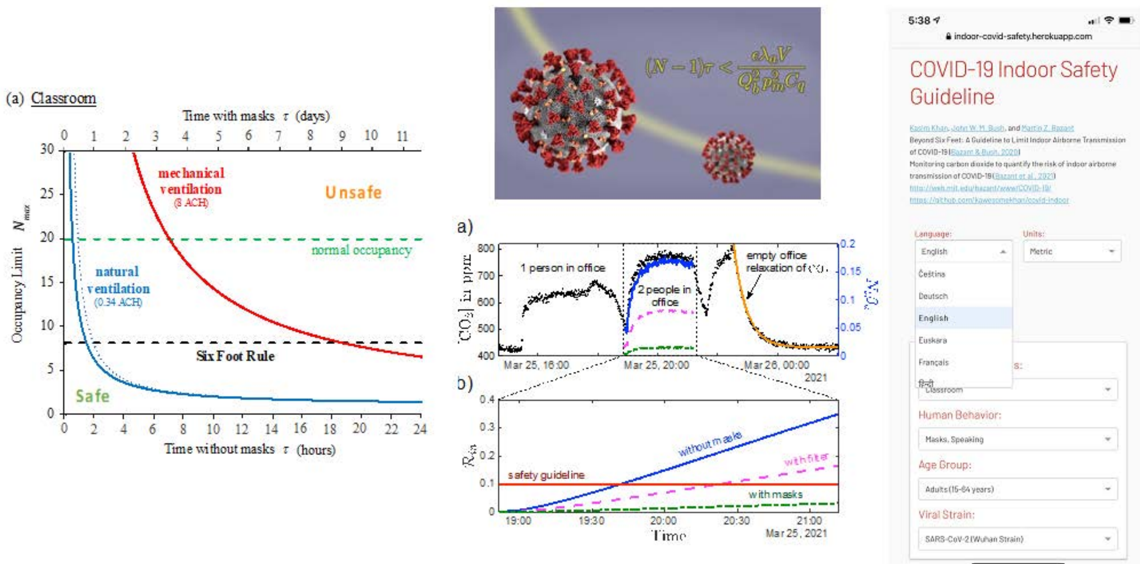


Figure 3. Left: sample calculation of the safety bound for a typical classroom, with and without a mask mandate. Middle: monitoring of excess carbon dioxide in an MIT office, converted to Covid-19 transmission risk in real time. Right: the online app in basic mode with simple pull-down menus and recommendations, which can be converted to advanced mode with detailed parameters and graphical outputs of safe CO_2 levels and time limits for a specific indoor space for a given population.

The guideline bounds the cumulative exposure time in an enclosed space depending on the rates of ventilation and air filtration, the dimensions of the room, breathing rate, respiratory activity, face mask use, and the infectiousness of exhaled air. Real-time monitoring of transmission risk can also be accomplished by expressing the guideline as a bound on safe carbon dioxide concentrations, which can be easily measured and used to optimize heating, ventilation, and air conditioning systems in buildings. A key to this work was to link experimentally measured droplet distributions from different respiratory activities to field data for super-spreading Covid-19 events and achieve conservative, quantitative predictions. We partnered with app developer Kasim Khan and produced a convenient and easy-to-use Covid-19 indoor safety guideline online app that our colleagues helped us translate into more than 20 languages. The app had around a million uses during the second wave of Covid-19 in fall 2020 and remains a standard reference. We also created a MOOC on edX, 10.S95x Physics of COVID-19 Transmission, and spent long hours on public outreach and advocacy for science-based policy decisions.

Designing Synthetic Membranes for an Energy-Efficient and Sustainable Chemical Industry (Zachary P. Smith)

Separation and purification of small molecules is accomplished using energy-intensive and thermally driven processes such as distillation. These processes account for roughly 10% to 15% of the world's energy consumption, and it has been estimated that more energy-efficient alternatives such as membrane-based separations would consume 90% less energy, saving 100 million tons of CO_2 and $4 billion annually in the United States alone. Unfortunately, membrane materials that exist today lack the separation performance and stability needed to replace traditional separation processes. Innovation is needed, and Professor Smith and his group focus on discovering and developing new materials to transform the field of molecular separations.

We are particularly interested in the use of polymers to address these challenges. Along these lines, we have been developing a research program that focuses on understanding the role of polymer chemistry and polymer morphology in separation performance. One intriguing functionality is fluorine, which exhibits anomalous and beneficial properties for various membrane-based separations when added to polymer backbones. We recently quantified the theoretical permeability and selectivity performance limits for fluorinated polymers, and we have developed synthetic techniques to form polyimides that are selectively fluorinated, enabling us to systematically study the role of incremental fluorine content in molecular transport. An example of two polymers we have investigated for selective fluorination, as well as our theoretical permeability-selectivity "upper bound" tradeoff, is highlighted in Figure 4.

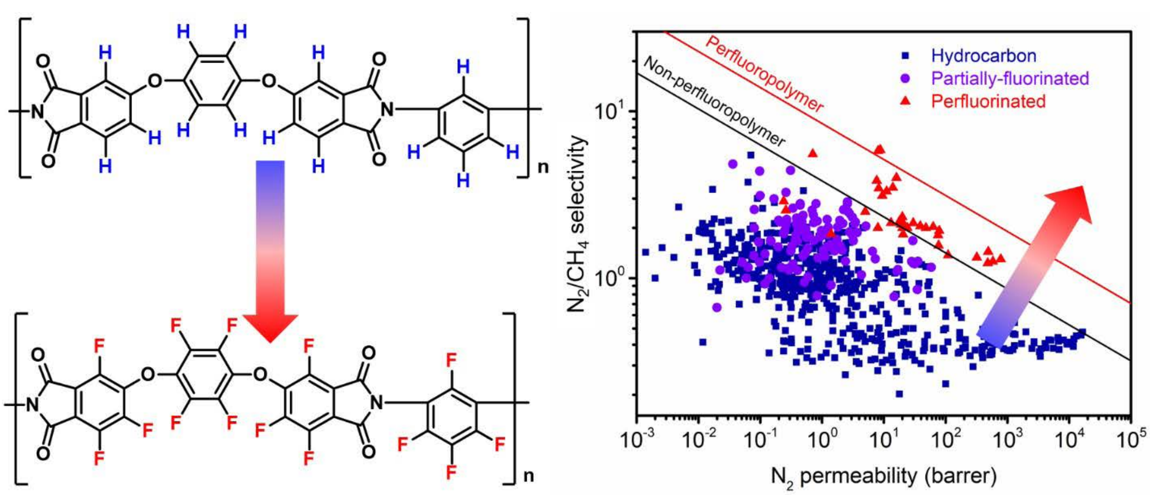


Figure 4. Designing polymers with fluorine functionality to surpass permeability-selectivity tradeoff limits for membrane-based gas separations.

In addition to fluoropolymers, the group has a significant interest in polymers of intrinsic microporosity (PIMs). This class of materials is unique among polymers in that it provides a solution-processable approach to making microporous membrane films with ultra-high permeabilities. Regrettably, traditional PIMs are unstable in complex mixtures and lose permeability over time, and there are very few accessible backbone chemistries and functional groups that can be formed into high molecular weight polymers. We have been developing improved synthetic methods to add CO_2-philic functionality to PIMs, and we have also discovered a method to template additional and stable porosity into these materials, which surprisingly improves mixed-gas selectivities. In addition, in collaboration with other research groups at MIT and Stanford, we have designed novel PIMs with traditional ladder-like structures or unique bottlebrush architectures that contain ladder side chains. The ladder side chain motif results in materials that are far more structurally stable than their linear analogues, potentially paving the way for these types of polymers to be applied to various separations in the chemical industry that cannot be accomplished using known membrane materials today. In other work, we have designed a new class of PIMs that surpass pure- and mixed-gas permeability and selectivity limits of all known polymers for certain gas separations by leveraging design principles to precisely contort polymer backbone geometry to form microporous size-screening domains that sieve molecules between 2.6 and 3.8 Å with selectivities that have never before been accessed.

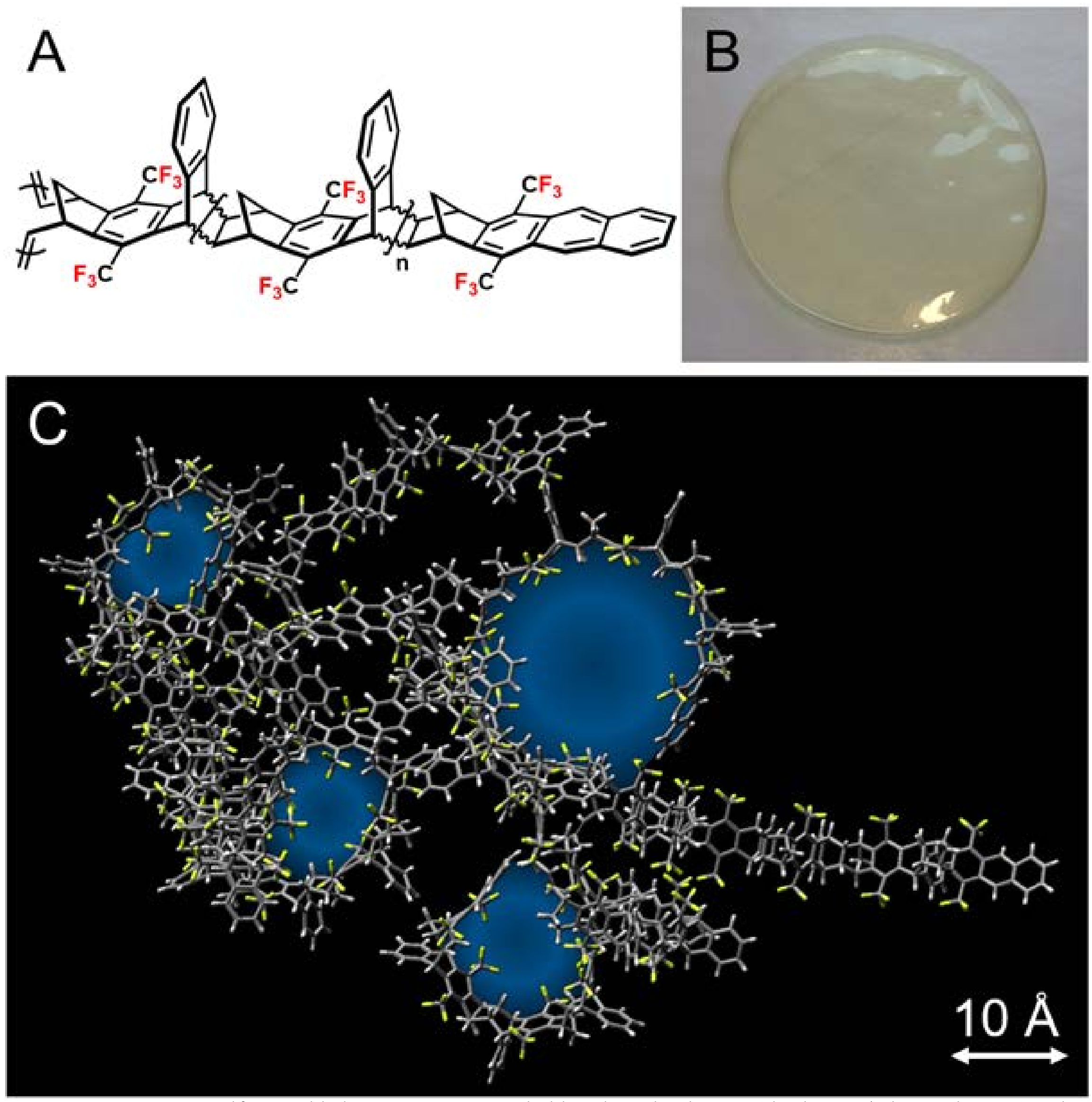


Figure 5. Generating self-assembled micropores using ladder-shaped polymer side chains: (A) two-dimensional polymer structure, (B) photo of the membrane film in the lab, and (C) three-dimensional polymer conformation highlighting (in blue) microporous domains.

Figure 5A shows one of the novel polymer structures we are investigating. It should be noted that we selected fluorinated functionality for the same reasons outlined in the text regarding Figure 4. In the lab, we developed methods to transform this exciting structure into a membrane film (Figure 5B), allowing us to collect experimental data on separation performance. Because of its well-defined microporous structure, highlighted through molecular dynamics simulations in Figure 5C, this polymer is capable of achieving some of the highest known CO_2 permeabilities while still maintaining selectivity to other gases. Access to these high permeabilities and selectivities makes this polymer particularly attractive in addressing issues related to CO_2 capture and biogas purification, processes that are considered critical for confronting global environmental and sustainability challenges.

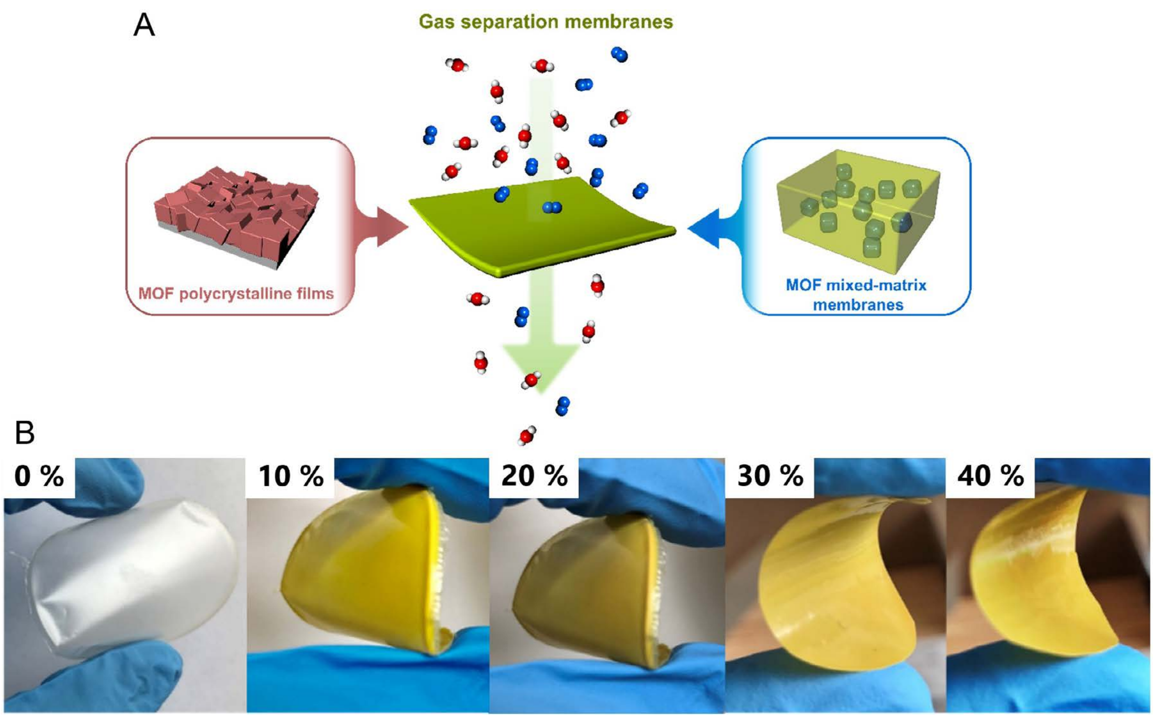


Figure 6. (A) Approaches to making new membrane materials in the Smith lab, including the development of MOF polycrystalline films and mixed-matrix membranes. (B) Example of forming MOF-polymer composite membranes with MOF loadings up to 40%.

In the coming years, we envision that the design strategies we have developed will enable us to make membrane materials and adsorbents to address many separation applications that we have just begun to consider, such as gas separations, vapor separations, water purification, dye filtration, protein separations, and solvent separations. Our work focuses on materials synthesis and characterization with the primary aim of applying chemical engineering principles to confront some of the major challenges of our day related to energy, sustainability, and the environment.

Annual Lectures and Seminars

Due to the Covid-19 pandemic, the department suspended the majority of its named lecture series. The weekly seminar series was held virtually, allowing the department to continue to host a distinguished group of academic and industry leaders speaking on topics highlighting cutting-edge research addressing today's energy and health-related challenges.

The 42nd Warren K. Lewis Lecture was delivered on May 6 by Howard A. Stone, Donald R. Dixon ’69 and Elizabeth W. Dixon Professor in Mechanical and Aerospace Engineering at Princeton University. In “Short Stories in Fluid Dynamics at Different Length Scales: (1) Speech and Spreading of a Pathogen, (2) Thin Films and a Novel Similarity Solution, and (3) Nanoscale Capillary Instabilities and Molecular Biology,” Professor Stone presented his thoughts on how many modern research themes in science and engineering introduce new questions, some of which can be at least partially understood using fundamental concepts. He provided several examples of his recent research combining experiments and theory at different length scales, from large to small. Professor Stone’s research interests are in fluid dynamics, especially as they arise in research and applications at the interface of engineering, chemistry, physics, and biology. He is a fellow of the American Physical Society (APS) and past chair of the APS Division of Fluid Dynamics. He received the 2016 APS Fluid Dynamics Prize and the 2008 G.K. Batchelor Prize in Fluid Dynamics.

Departmental Awards

The department’s awards ceremony took place virtually on May 17, 2021, in conjunction with our online (via Zoom) commencement celebration. We are pleased to recognize this year’s recipients of the Outstanding Faculty Awards: Arup Chakraborty was the graduate students’ choice, and William Tisdale was selected by the undergraduate students.

The Edward W. Merrill Outstanding Teaching Assistant Award was presented to graduate students Haberly Kahn for 10.37 Chemical Kinetics and Reactor Design, Haley Beech for 10.467 Polymer Science Lab, Supratim Das for 10.493 10.493 Integrated Chemical Engineering Topics II IAP, and Amber Phillips for 10.10 Introduction to Chemical Engineering. PhD student Aditya Limaye won the Outstanding Graduate Teaching Assistant Award for his work in 10.40 Chemical Engineering Thermodynamics. All third-year graduate students are required to present a seminar on the progress of their research, and the two recipients of the Award for Outstanding Seminar were Kevin Tenny and Bertrand Neyhouse.

Chemical Engineering Special Service Awards were conferred to the members of the Graduate Student Council: Amanda Farnsworth, Aristotle Grosz, Blake Johnson, Christopher Johnstone, Daniel Chu, Debbie Zhuang, Grant Knappe, Kevin Greenman, and Rose Yin. Members of the Graduate Student Advisory Board were also recognized: Alexander Khechfe, Amber Phillips, Bertrand Neyhouse, Brianna Lax, Eric Powers, Katherine Steinberg, Kindle Williams, Mary Joens, Thejas Wesley, James Owens, Wei Han Lim, and Kara Rodby. Members of the Graduate Women in Chemical Engineering group were recognized as well: Kara Rodby, Jennifer Kaczmarek, Junli Hao, Haley Beech, Katharine Greco, Katherine Steinberg, Kaylee McCormack, Kelsey Reed, Madeline Dery, Maylin Howard, Narumi Wong, Sarah Cowles, Stephanie Kong, Tam Nguyen, and Yining Hao. In addition, awards were given to the following members of the Resources for Easing Friction and Stress group: Kevin Silmore, Cynthia Ni, MayLin Howard, Jennifer Kaczmarek, Joy Zeng, Chun Man Chow, Cindy Jin, Emily Krucker-Velasquez, Pradeep Natarajan, Srinivasa (Srinu) Pujari, and Jessica Xu. Finally, members of Diversity in Chemical Engineering were recognized: Alexander Quinn, Cynthia Ni, Emily Stephanie Krucker-Velasquez, Grant Knappe, Joseph Maalouf, K'yal Bannister, Kindle Williams, Madeline Dery, Mary Joens, Kyle Diederichsen, and Sydney Johnson.

The Michael Johnson Award went to Eliza Price. Kevin Greenman and Kindle Williams received the Chemical Engineering Rock Award for their contributions to athletic achievement within the department.

The following undergraduate students were recognized for their service to the student chapter of AIChE: Caroline Kenton, Kara Zhang, Danica Dong, Britney Pham, Daiyao Zhang, Ashleigh Teygong, Ming Yang, Nicole Munne, Ruoxin Lu, Julie Tung, Shuxin Chen, Sydney Vleck, Jacky Chin, Evan Gwozdz, Paula Pieper, Binette Wadda, Seraphin Castelino, and Andison Tran. Also recognized were the officers of the student chapter of NOBCChE: Lina Ahmed and Asia Hypsher. Other service awards went to the officers of the Undergraduate Student Advisory Board: Andrea Orji, Daiyao Zhang, Freya Edholm, Julie Tung, Nicole Munne, Victoria Yang, and Zachary Villaverde.

Our undergraduates earned numerous accolades over the course of the year. The Robert T. Haslam Cup, which recognizes outstanding professional promise in chemical engineering, went to Zachary Villaverde. The department's oldest prize, the Roger de Friez Hunneman Prize, is awarded to an undergraduate who has demonstrated outstanding achievement in both scholarship and research; this year's winner was Rais Aoudou. The Lourdes C. and Wing S. Fong Memorial Prize, awarded to a chemical engineering senior of Chinese descent with the highest cumulative GPA, went to Daiyao Zhang, Jacky Chin, and Stefan Wan. The 2021 Phi Beta Kappa electees were Jacky Chin, James Drayton, and Daiyao Zhang.

We are pleased to recognize James Hardsog as the department's Outstanding Employee of the Year for his dedication and exceptional service to faculty, staff, and students. Chemical Engineering Individual Accomplishments Awards were presented to Helen Arroyo, Adrienne Bruno, Sharece Corner, Leposava Gagoska, Caroline Kenton, Chris Monaco, Bertrand Neyhouse, Kristala Prather, Brian Smith, Matthew Sweeney, Beth Tuths, Cindy Welch, and Gwen Wilcox. The Chemical Engineering Diversity, Equity, and Inclusion Awards, presented for the first time, went to undergraduate student Asia Hypsher, graduate student Madeline Dery, and staff member Sharece Corner.

Paula T. Hammond
Department Head
David H. Koch Professor of Chemical Engineering

Kristala L. J. Prather
Executive Officer
Arthur D. Little Professor of Chemical Engineering