Department of Chemical Engineering

Overview

During academic year 2017–2018, the Department of Chemical Engineering maintained its global leadership in the field. For the 29th straight year, our undergraduate and graduate programs were both ranked number one by *US News & World Report*. The department was also ranked number one in the QS World University Rankings for chemical engineering for the fifth consecutive year and contributed to the record-breaking seventh straight year that MIT was ranked first among world universities overall. This position is maintained in the context of an increasingly competitive chemical engineering landscape in which some peer institutions have grown considerably over the past several years.

Sponsored research volume in the department has remained healthy, at $56.9 million; $22.2 million of these funds were handled directly through the department and the remainder by different cost centers at MIT, such as the Koch Institute for Integrative Cancer Research, the MIT Energy Initiative (MITEI), and the Ragon Institute. Our faculty members continue to attract significant funding for their individual research while strongly engaging with these interdisciplinary centers and contributing to the creation and direction of numerous multi-investigator research centers.

Our department continues to play a major role in three manufacturing innovation institutes. The institutes are nonprofit corporations initially funded for five years through $70 million in support from the US Department of Energy (DOE), with a total of $140 million in project spending including the institutes' extensive networks of national industrial partners. Professor Richard D. Braatz led MIT's contribution to the Clean Energy Smart Manufacturing Innovation Institute (CESMII), which aims to develop sensors, high-fidelity simulations, and data analytics for advanced manufacturing. Professor Michael Strano serves as MIT's contact with the Rapid Advancement in Process Intensification Deployment (RAPID) Manufacturing Institute, a DOE-sponsored institute administered by the American Institute of Chemical Engineers (AIChE). MIT officially became a member of RAPID in May 2018 and has participated in workshops, strategic planning, and workforce development efforts. Professor Gregory C. Rutledge is the lead MIT principal investigator (PI) for Advanced Functional Fabrics of America (AFFOA), a manufacturing innovation institute created in 2016 and headquartered in Cambridge; this institute has been awarded $75 million in funding over five years from the US Department of Defense (DOD), with additional funding from the state of Massachusetts. AFFOA's mission is to enable a manufacturing-based revolution in fibers, yarns, and fabrics as integrated and networked devices and systems. Also, Professor Braatz continued to serve as MIT's representative to and as a director of the Smart Manufacturing Leadership Coalition (SMLC), a private-public partnership that is building the first open smart manufacturing platform for collaborative industrial-networked information technology applications. SMLC is the nonprofit organization that manages the operations of CESMII.

The 2017–2018 year brought new student services offered by the department for the first time. The new Chemical Engineering Communication Lab, launched in summer 2017,

just completed a very successful first year, with high usage among both undergraduate and graduate students. The lab's communications fellows (peer graduate students and postdocs) assist students with technical writing and communications, to greatly enhance the ability of students to communicate their ideas in professional settings. The lab's career development manager serves as a highly effective conduit between industry and students in the department.

Professor Paula T. Hammond completed her third year as department head, and Professor Bazant completed his second year as executive officer. In July 2017, Professor Patrick Doyle returned from sabbatical to his former position as graduate officer. Professor Bill Green completed his third year as postdoctoral officer, and Barry Johnston continued his long service as undergraduate officer. Professor T. Alan Hatton remains the director of the David H. Koch School of Chemical Engineering Practice. Chemical Engineering continues to claim two Institute Professors as primary faculty members—Daniel I.C. Wang and Robert S. Langer. Professor Robert C. Armstrong is the director of the MIT Energy Initiative. Professor Arup K. Chakraborty stepped down from his role as the founding director of the MIT Institute for Medical Engineering and Science (IMES) in January 2018. Also, Professor Dane Wittrup stepped down from his long-standing role as associate director of the Koch Institute for Integrative Cancer Research in September 2017, and Professor Karen Gleason recently stepped down as associate provost.

Promotions, Staffing Changes, and Retirements

J. Christopher Love was promoted to full professor, and Fikile Brushett was promoted to associate professor without tenure. The Administrative Services Organization, which previously supported the department in both human resources and finance, was dissolved during summer 2017. The new organization supporting the department is Chemical Engineering Administrative Services, and it retained many of the former organization's staff to continue supporting human resources and finance functions. Brian Tavares was appointed administrative officer as of September 1, 2017. Professors Robert Cohen and Preetinder Virk retired to emeritus status, and George Stephanopoulos became professor post-tenure.

Recognition and Research

Several members of the Chemical Engineering faculty received major awards for their research achievements. For example, Klavs Jensen was named AIChE's 2018 John Prausnitz Institute Lecturer and received the 2018 Corning International Prize for Outstanding Work in Continuous-Flow Reactors and Chemistry for a Greener and Safer World. Heather Kulik received the DARPA (Defense Advanced Research Projects Agency) Young Faculty Award, the ACS OpenEye Outstanding Junior Faculty Award, and the Office of Naval Research Young Investigator Award. Robert Langer was named a US science envoy, won the 2017 Kabiller Prize in Nanoscience and Nanomedicine, and once again topped the Medicine Maker Power List. Zachary Smith was presented a DOE Early Career Award, received an MIT Abdul Latif Jameel Water and Food Systems Lab (J-WAFS) grant for work in water purification, and was named an ACS Petroleum Research Fund Doctoral New Investigator.

Alan Hatton, Jesse Kroll, and Greg Stephanopoulos won Tata Center grants. Paula Hammond, Brad Olsen, and Hadley Sikes earned MIT's 2018 Committed to Caring

Award. Bill Green and Janos Beer were named inaugural fellows of the Combustion Institute. Kulik and Sikes won CEHS grants. Karthish Manthiram was named to the *Forbes* 30 Under 30 list and earned a J-WAFS seed grant for his work on a more efficient way to produce nitrogen fertilizer. Yuriy Roman won the 2018 Robert Augustine Award. Kulik and Fikile Brushett were named influential researchers by *I&EC Research*.

It was an exciting year of research for the department, with many new developments coming out of Chemical Engineering laboratories. Michael Strano's lab developed cell-sized robots that can sense their environment, store data, and carry out computational tasks and a model that predicts the performance of glucose-responsive insulin. In addition, his lab created "artificial blubber" insulated wetsuits, technology that harnesses external temperatures to produce electricity, sensors that allow a plant to warn of water shortage, and plants that glow. Dan Anderson developed nanoparticles to improve delivery of therapeutic messenger RNA and found a way to improve the life span of implanted devices. Karen Gleason and colleagues created coatings to make natural fabrics waterproof and turned a plastic insulator into a heat conductor.

Patrick Doyle's lab discovered how to control knots that form in DNA molecules. Clark Colton and colleagues developed an implantable device to improve treatment of type 1 diabetes. Robert Langer's lab used caffeine to create new gels for drug delivery, created ultra-thin needles to deliver drugs directly to the brain, enhanced ingestible drug-delivery materials, and developed a single-injection vaccine for polio. Also, Langer developed 3D fabricated microparticles that allow multiple drug doses to be delivered in one vaccine. Paula Hammond and her lab designed brain-tumor-targeting nanoparticles that can carry two drugs, crossing the blood-brain barrier and shrinking glioblastoma tumors. Hammond also developed a new technique that could make it easier to use mRNA to treat disease or deliver vaccines. Chris Love helped develop new techniques that give blood biopsies greater promise and a portable tool that makes single-cell RNA sequencing widely available. William Tisdale's lab developed novel methods of synthesizing quantum dot materials for energy devices. Greg Rutledge's new ultra-fine fibers were found to have exceptional strength. Martin Bazant published a mathematical theory predicting how viscous fingering (the notorious and prototypical instability of two-phase fluid flow) can be controlled by applied electric fields.

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

Undergraduate Education

Since 2004, the Department of Chemical Engineering has offered bachelor of science (SB) degrees in both chemical engineering (Course 10) and chemical-biological engineering (Course 10-B). In fall 2011, we introduced the 10-ENG flexible SB degree in engineering. Department undergraduate enrollment has been gradually declining since AY2007, but Chemical Engineering continues to have one of the highest student-to-faculty ratios in the School of Engineering. The department advises students about career paths in chemical and chemical-biological engineering through active participation in freshman advising seminars, fall and spring term open houses, Family Weekend, and other activities. Forty-nine SB degrees were conferred in June 2018, 57% of which were

awarded to women. Student quality remains high. The distribution of undergraduate students by class over the last 13 years is shown in Table 1.

Table 1. Undergraduate Enrollment over the Last 10 Years

Class year	08–09	09–10	10–11	11–12	12–13	13–14	14–15	15–16	16–17	17–18
Sophomores	87	87	80	72	61	67	57	56	58	44
Juniors	77	68	71	73	63	63	66	53	51	53
Seniors	75	73	75	75	69	58	64	67	55	50
Total	**239**	**228**	**226**	**220**	**193**	**188**	**187**	**176**	**164**	**147**

The 10-ENG program leading to the engineering bachelor of science degree was introduced in response to demand from our students for a curriculum that would allow specialization in particular topics. The program features some flexibility in that requirements of the Department, the Institute, and the profession may be met in some cases by categories of subjects rather than particular subjects. We have recently received ABET accreditation for 10-ENG as a degree in engineering. The initial specialization tracks are energy, materials, biomedical, and environmental. Student response has been cautious (with a fall 2017 enrollment of seven students).

The average starting salary for graduates of the Department of Chemical Engineering is $105,429 (2018 senior survey), which is among the highest in the School of Engineering. This attests to the success of the graduates of the 10 and 10-B programs and to the continued high demand for our students. The senior survey indicates that 35% 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 Andrea Blankenship, Marjorie Buss, Sarah Coleman, Natalie Delumpa-Alexander, Erika Ding, Anj Fayemi, Michelle Huang, Morgan Matranga, Rafid Mollah, Linh Nguyen, Luis Sandoval, Zach Schmitz, Amy Wang, Nancy Wang, Emily Yan, and Brian Zhong.

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 226, with 214 in the doctoral program and 12 master's-level degree candidates. In the doctoral program, 207 students are in the PhD/ScD track and seven in the PhDCEP track. In the master's-level program, 10 students are in the MSCEP track. Twenty-nine percent of our graduate students are women, and 4% are members of underrepresented minority groups. Forty-nine of our

graduate students were recipients of outside fellowship awards, including awards from the National Science Foundation (NSF), the National Institutes of Health, and DOD. The distribution of graduate students by degree level over the last 11 years is shown in Table 2. During AY2018, 64 advanced degrees were conferred, 32 each at the doctoral level (PhD, ScD, PhDCEP) and master's level (MSCEP, MS).

The department received 476 applications for admission to the doctoral program and offered admission to 60 individuals; 42 students accepted the offer (an acceptance rate of 70%). There were 92 applications for master's-level programs; the department made eight offers, all of which were accepted. Among the incoming graduate class, 15 students are women and two are members of underrepresented minority groups. The average GPA of the incoming graduate class was 3.97 (out of 4.0).

Table 2. Graduate Enrollment over the Last 10 Years

Degree level	08–09	09–10	10–11	11–12	12–13	13–14	14–15	15–16	16–17	17–18
Master's	32	38	28	20	10	11	15	15	10	12
Doctoral	228	203	212	224	212	211	222	218	222	214
Total	**260**	**241**	**240**	**244**	**222**	**222**	**237**	**233**	**232**	**226**

Research Centers

The Department of Chemical Engineering is actively involved in 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.

Biologically Derived Medicines on Demand

Today's manufacturing solutions for biologic medicines are not well aligned with emerging interests in precision medicine that rely on improved stratification of diseases based on molecular profiles. A DARPA-sponsored program called Integrated Scalable Cyto-Technology (InSCyT) aims to establish an end-to-end manufacturing system for making small batches of recombinant biologic therapeutics in a few days at or near the point of care. The program team, led by Professor J. Christopher Love of the Koch Institute, emphasizes small-scale continual production and purification, incorporating concepts of quality by design, process analytics, plant-scale control, and real-time release. In the past year, the team has extended its prototype systems to produce dozens to thousands of purified doses of different biologic drugs that have attributes comparable to those of existing commercial products. The ability to make biologic drugs at small scales anywhere could substantially improve precision medicine, including addressing rare and orphan diseases, and potentially lower the costs of supplying these drugs.

The objectives of this project are ambitious. Today, manufacturing biologics requires weeks to months for production and release, using many separate operations often spread physically across global facilities. To allow a system more akin to a 3D printer in capability, we have developed a benchtop-sized manufacturing system designed to be portable and flexible and to create many different high-quality therapeutics for patients.

The interdisciplinary research team comprises labs in Chemical Engineering at MIT (Professors Braatz and Love) as well as labs from the Barnett Institute at Northeastern University (Professor William Hancock) and the Rensselaer Polytechnic Institute (Professor Steven Cramer). Research topics include small-scale perfusion fermentation of a yeast host, novel purification strategies, and systems control strategies. An essential element of the program is integration of technologies to realize an efficient and small manufacturing platform that can be portable enough to reach remote locations. Examples of high-quality products made to date include human growth hormone, used to treat growth disorders in pediatrics, and two common cancer therapeutics (interferon alpha and G-CSF). Significant advances in biological understanding of the microbial host, process intensification, and system operations have increased both the productivity and the quality of the proteins made. With additional project financial support, the team has constructed a complete next-generation prototype designed for aseptic operations. Success in this program has also led to a related new Grand Challenges project, sponsored by the Bill and Melinda Gates Foundation, focusing on ultra-low-cost large-scale vaccine manufacturing; the project, led by Professor Braatz, Associate Professor Kripa Varanasi (Department of Mechanical Engineering), and Professor Love, is being conducted in collaboration with University College London and Kansas University.

Novartis-MIT Center for Continuous Manufacturing

May 2018 marked the end of the 11th year of a now 12-year collaboration with Novartis on continuous manufacturing of pharmaceuticals. We have continued to work on a large set of projects to overcome technical problems related to the transition from batch manufacturing to the more efficient continuous mode. This work has been conducted in 12 research groups spread across three departments (Chemical Engineering, Chemistry, and Mechanical Engineering).

Although we are working closely with Novartis on the projects, the advances and findings have been published in a wide variety of journals and new intellectual property has been captured in patents. In the last year alone, project researchers published over 30 papers and the center filed several patent applications for breakthrough technologies.

We not only have made great strides in solving the technical problems related to continuous manufacturing of complex and high-value drug molecules but have also engaged the global pharmaceutical industry, academics, and regulators to attack regulatory and mind-set challenges to adoption. For example, we are jointly organizing the third International Symposium on Continuous Manufacturing of Pharmaceuticals, which will be held in London. Janet Woodcock, head of the Center for Drug Evaluation and Research of the Food and Drug Administration (FDA), will present the keynote address. The meeting will bring together global leaders in the pharmaceutical world to report on the advances made in the past two years and to discuss remaining challenges. Among the major outputs of the symposium will be white papers on continuous manufacturing of pharmaceuticals.

The center is led by director Bernhardt L. Trout and Novartis head of continuous manufacturing Markus Krumme.

Disruptive and Sustainable Technology for Agricultural Precision

In January, Professor Michael Strano held the kickoff meeting for DiSTAP (Disruptive and Sustainable Technology for Agricultural Precision), a $40 million effort for which he is the lead PI. This new Singapore-MIT Alliance for Research and Technology (SMART) interdisciplinary research group (IRG), based in part on Strano's recent advances in plant nanobionics, focuses on new technology for urban farming and biomanufacturing to advance food security. Professor Gregory Stephanopoulos is a DiSTAP co-PI focusing on the biosynthesis of hydrophobic vitamins. Professor Strano is also the lead PI for an MIT-centered Engineering Frontier Research Center, called CENT (Center for Nanofluidic Transport), that involves seven universities and the Lawrence Livermore National Laboratory. This $11 million DOE-sponsored center will investigate new physical phenomena observed in single-digit nanopores, or pores below approximately 10 nm in diameter, where fluid properties and molecular transport exhibit exotic behavior. These efforts promise new mechanisms of chemical separation and water purification. MIT co-PIs Martin Bazant, Heather Kulik, and Daniel Blankschtein will lead CENT molecular simulation, quantum chemistry, and theory efforts.

David H. Koch Institute for Integrative Cancer Research

Five Chemical Engineering research laboratories are housed in the David H. Koch Institute for Integrative Cancer Research: those of Daniel Anderson, Paula Hammond, Robert Langer, Christopher Love, and Dane Wittrup. The Koch Institute brings together scientists and engineers with appointments spanning the campus to collaborate on research aimed at new cancer therapies. Wittrup serves as the institute's associate director. A particular strength of the Koch Institute is cutting-edge research on drug delivery, anchored by the efforts of Anderson, Hammond, and Langer.

Other Projects

Professors Klavs Jensen and Allan Myerson continued to lead the DARPA Pharmacy on Demand Project, which involves the development of a tabletop pharmaceutical manufacturing device, while Professors Jensen, Myerson, and Braatz continued another DARPA project, Make-It, which involves automated robotic chemical synthesis combined with computational synthesis design integrating machine learning, computational chemistry, and retrosynthetic tools for reaction pathway identification and selection.

With colleagues in the Computer Science and Artificial Intelligence Laboratory (Professors Regina Barzilay and Tommi Jaakkola) and the Department of Chemistry (Professor Timothy Jamison), Professors Jensen and Green initiated the new MIT-industry Machine Learning for Pharmaceutical Discovery and Synthesis Consortium. The consortium includes eight industry partners, all major players in the pharmaceutical field: Amgen, BASF, Bayer, Lilly, Novartis, Pfizer, Sunovion, and WuXi.

Faculty Notes

Robert C. Armstrong serves as director of the MIT Energy Initiative. MITEI continues to grow rapidly in its research, educational, and outreach components. Eleven companies sponsor research as founding, sustaining, and start-up members of MITEI. We are particularly excited about our newest start-up member, Commonwealth Fusion Systems,

whose technology may truly revolutionize the world's energy systems. Altogether, the energy initiative has more than 80 industrial and public partners and individual members across four continents. MITEI has helped to bring in over $700 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, announced in 2015 as key components of MIT's climate action plan, continue to develop. MITEI continued the Mobility of the Future Study and launched the Future of Storage Study, the latest in a series of multi-faculty, multidisciplinary studies aimed at informing discussions between industry and policymakers around the role of key technologies in meeting future energy demand growth in a carbon-constrained world. Professor Armstrong serves on the scientific commission of the Eni Enrico Matteo Foundation, the editorial board of *World Energy* magazine, and the external advisory committee of the National Renewal Energy Laboratory. Also, he serves on the advisory boards of the chemical engineering departments at Northwestern University and Washington University and the Energy Institute at Texas A&M University. He presented numerous lectures on energy around the world during the past year.

Martin Z. Bazant continued research in electrochemistry, transport phenomena, and applied mathematics while completing his second year as the department's executive officer. He won a grant from MITx to develop the first graduate-level MOOCs (massive open online courses) on EdX in chemical engineering and applied mathematics. The first of two 10.50x Analysis of Transport Phenomena modules is scheduled to run for the first time in fall 2019, and four modules of 18.075x Mathematical Methods for Scientist and Engineers and a companion textbook are also planned. Professor Bazant published more than 15 papers, including one describing a mathematical theory of the electrokinetic control of viscous fingering. His group also published numerous papers on multiscale battery modeling, as well as an open-source software package, Multiphase Porous Electrode Theory. He completed his first year as director of D3BATT (Data-Driven Design of Rechargeable Batteries), a $6 million Toyota Research Institute center,. He also continued to serve as chief scientific advisor for Saint-Gobain North America. He delivered 10 invited talks at conferences and universities and was named a fellow of the Royal Society of Chemistry. In addition, he was selected to receive the 2018 Andreas Acrivos Award for Professional Progress in Chemical Engineering, AIChE's highest mid-career honor.

Daniel Blankschtein's group conducts fundamental theoretical and experimental research in the area of colloid and interface science, with an emphasis on industrial and biomedical applications. Recent research advances include molecular dynamics simulation of the exfoliation, dispersion, and stabilization of 2D materials such as MoS2 and hBN in various solvents; molecular modeling of the wetting behavior of water and other solvents on graphene, MoS2, and hBN; molecular-thermodynamic modeling of the surface tension of aqueous surfactant solutions; modeling and experimental studies of gas separation and water desalination using carbon nanotubes and 2D porous membranes; multi-scale approaches to model stability, aggregation, and network formation of nanoparticles suspended in aqueous solutions; and ultrasound-assisted transdermal vaccination. Professor Blankschtein interacts with several companies that make use of software developed by his group to facilitate surfactant formulation design. His group presented invited talks, regular talks, seminars, and posters at the 91st ACS Colloid & Surface Science Symposium in New York, the 2017 Materials Research Society fall meeting in

Boston, the 255th ACS national meeting in New Orleans, and the 22nd International Symposium on Surfactants in Solution in Norman, OK. Professor Blankschtein continues to serve on the editorial board of Marcel Dekker's Surfactant Science Series.

As the department's faculty research officer, Richard D. Braatz facilitated strategic planning and informed faculty of potential opportunities in national manufacturing innovation institutes. One of his theoretical journal papers was selected for the Automatica Paper Prize, which is awarded for "outstanding contributions to the theory and/or practice of control engineering or control science." Professor Braatz continued to lead systems engineering research in several large advanced manufacturing projects on campus. In addition, he was the president of the American Automatic Control Council, served on several advisory and editorial boards, and gave numerous invited lectures, including plenaries and keynotes.

Fikile R. Brushett was promoted to associate professor without tenure effective July 1, 2018, and now holds the Green Career Development Chair, which is presented to recognize and encourage excellence in teaching. His research group continued its work advancing the science and engineering of electrochemical systems for energy storage and conversion. Major accomplishments included the development of inexpensive sulfur-based aqueous flow batteries for grid storage as well as the demonstration that, contrary to popular belief in the energy storage community, low resistance nonaqueous flow batteries can be engineered. This research is supported by DOE, NSF, the Deshpande Center for Technological Innovation, Shell, Exxon Mobil, and the MIT Energy Initiative. In addition, collaborative work is being initiated with a number of companies in the chemical manufacturing and electrochemical technology space. In the past year, Brushett has published 10 peer-reviewed papers and has given 14 invited lectures. He was recognized for his scholarship by being named to *Chemical & Engineering News*'s Talented 12 list, being appointed a Scialog Fellow in Advanced Energy Storage, and being named a finalist for the BASF Volkswagen Science Award Electrochemistry. He serves on the scientific advisory board at Form Energy.

Arup K. Chakraborty continued efforts to understand the mechanistic bases of how a specific and systemic immune response to pathogens occurs and how its aberrant regulation leads to disease. Research aimed toward 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, launched a new project on understanding how genes critical for maintaining healthy cell states are regulated. Chakraborty is also working on two books on immunology, one targeting physical scientists and one intended for a general audience. Chakraborty served as the director of IMES until December 31, 2017, and co-chaired MIT's Committee on Digital Health. He continues to serve as a member of the US Defense Science Board and as a senior editor of *eLife* (one of the premier journals in biology). In 2017, Chakraborty was elected a member of the National Academy of Medicine, making him one of only 21 individuals who are members of all three National Academies (Science, Engineering, and Medicine). He also received a Guggenheim Fellowship in 2018.

Charles L. Cooney, Robert T. Haslam (1911) Professor of Chemical and Biochemical Engineering (emeritus), teaches 10.491 Integrated Chemical Engineering, which

introduces all chemical engineering seniors to batch processes through the design of a manufacturing facility for therapeutic monoclonal antibodies. In addition, he 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, and co–faculty lead on a custom Sloan executive education program for Takeda Pharmaceuticals. Professor Cooney is also a member of the board of the Norman B. Leventhal Map Center at the Boston Public Library, an overseer emeritus of the Boston Symphony Orchestra, and a trustee emeritus of the Boston Ballet.

Patrick S. Doyle, Robert T. Haslam (1911) Professor of Chemical Engineering, returned from sabbatical and stepped back into the role of graduate officer for the department. His research continues to focus on soft matter, including fundamental studies of DNA polymer physics and microfluidic synthesis of functional microparticles. A significant study from his group published in *Physical Review Letters* showed the diverse dynamics of knots on single DNA molecules and provided conclusive evidence of jammed knot states. Along with department alumnus Saif Khan, he was awarded an Intra-CREATE grant in Singapore to conduct research in the area of advanced manufacturing of pharmaceutical drugs using modular microfluidic processes. His MIT spinout company Motif Micro was acquired by YPB Systems. He delivered several invited lectures at company meetings, conferences, and universities. Professor Doyle currently serves on the scientific advisory boards of Lariat Biosciences and Achira Labs.

William H. Green was named one of the 125 inaugural fellows of the Combustion Institute, the global society that sponsors the leading conferences and journals in combustion research. Professor Green presented an invited plenary lecture at the 117th annual meeting of the Bunsen Society, the theme of which was "Kinetics in the Real World." Green's research into methods for predicting and determining the rates and products of complicated reacting systems, including computer discovery of unexpected reactions and computer design of effective reaction sequences for organic synthesis, was very fruitful, leading to more than 20 journal papers published in the last 12 months. Several of these papers demonstrated that it is now feasible to accurately predict reactive chemistry on a computer prior to doing any experiments, even when the chemistry is rather complex and non-intuitive. This has the potential to dramatically change the practice of chemical engineering. In addition to his work on chemical reactions and kinetics, Professor Green continues as the faculty chair of MIT's Mobility of the Future consortium and as the department's postdoctoral officer. This year he was appointed chair of the Institute's Faculty Postdoctoral Advisory Committee.

During the 2017–2018 academic year, Department Head Paula Hammond focused on continued support of the department's efforts in undergraduate curricular reform while gathering input from our new Undergraduate Student Advisory Board on ways to improve the undergraduate experience. This year Professor Hammond was recognized with the American Chemical Society Award in Applied Polymer Science, which was presented during the organization's spring 2018 meeting. She was officially inducted into the National Academy of Engineering and the National Academy of Medicine in October 2017. Over the past year, she presented the Berkeley Lectures at the University of California, the John D. Ferry Lecture in Physical Chemistry at the University of Wisconsin,

and the Kurt Wohl Memorial Lecture at the University of Delaware. She was also invited to give a lecture as part of the Miller Symposium, held at the University of California, Berkeley. She gave the plenary opening talk at the 2018 IUPAC (International Union of Pure and Applied Chemistry) Polymer World Congress in Australia and a plenary address at the Bordeaux Polymers Conference. Professor Hammond continues to serve as associate editor of the American Chemical Society journal *ACS Nano*, and this year she joined the scientific advisory board of Moderna Therapeutics. Her research continues to focus on the areas of targeted cancer nano-therapies and immuno-oncology, wound healing, and tissue regeneration, with new technologies also directed toward infectious disease, emergency field care medicine, and targeted delivery treatments for osteoarthritis.

As noted, T. Alan Hatton continued to serve as the director of the David H. Koch School of Chemical Engineering Practice. In addition, he 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. During the past year, Hatton held an honorary professorial fellow appointment at the University of Melbourne and an adjunct professorship at Curtin University in Perth, Western Australia. He is an advisory board member of Engineering Conferences International in New York and a member of the Eni-MITEI steering committee. He presented invited lectures at various professional society meetings and a plenary keynote lecture at the Turin "CO2 Reduction in the Transport Sector" Conference.

Klavs F. Jensen conducted research on continuous flow synthesis and separation as part of the Novartis-MIT Center for Continuous Manufacturing and the DARPA-sponsored Pharmacy on Demand and Make-It programs. The Pharmacy on Demand effort, in collaboration with Professor Timothy Jamison and Professor Myerson, has moved from the initial demonstration of end-to-end synthesis of seven different pharmaceuticals toward technology that could be approved by the FDA. With colleagues in chemical engineering, chemistry, and computer science, Jensen worked on the DARPA Make-It program to develop machine learning algorithms for planning organic synthesis and to create a robotic system for automated chemical synthesis. Also, Jensen's lab continued its efforts to use automated platforms to optimize chemical reactions and extract chemical kinetics. In the area of materials synthesis, Jensen explored growth mechanisms underlying the formation of quantum dots. During the past academic year, he gave plenary lectures on microfluidics and microreaction technology at universities and international conferences and served on the scientific advisory boards of chemical engineering departments, research institutes, and companies. Professor Jensen received the inaugural Corning International Prize for Outstanding Work in Continuous-Flow Reactors and Chemistry for a Greener and Safer World, and he was inducted into the National Academy of Sciences.

Jesse H. Kroll and his research group continued their work on the organic chemistry of the atmosphere, the formation of atmospheric particulate matter, and distributed air quality measurements. A specific focus of their research has been comprehensive measurements of atmospheric carbon, the initial results of which were published in *Nature Geoscience* and *Nature Chemistry*. The group also continued its work on low-cost air quality sensing, expanding its efforts in Boston, Delhi, and Hawaii (where air quality was dramatically affected by the recent Kilauea eruption). Professor Kroll's

other activities in 2017–2018 included presenting several invited lectures, organizing conferences and workshops in atmospheric chemistry, and serving as graduate officer for the Department of Civil and Environmental Engineering.

Heather J. Kulik's group carries out interdisciplinary research in computational first-principles modeling for accelerated inorganic design and large-scale, predictive modeling of catalyst (both biological and nonbiological) and materials properties. Major accomplishments included the first practical no-cost recovery of high-accuracy conditions in electronic structure theory for modeling transition metal chemistry and accelerated discovery of functional transition metal materials through new approaches driven by machine learning. This past year, Professor Kulik received the ACS OpenEye Outstanding Junior Faculty Award in Computational Chemistry, the Office of Naval Research Young Investigator Award, and the DARPA Young Faculty Award. She traveled extensively, presenting over 20 talks in the past year at national and international universities and conferences. She published 13 peer-reviewed papers during 2017–2018, including a *Journal of Chemical Theory and Computation* editors' choice piece and a *Journal of Physical Chemistry Letters* article that was featured in *Chemical & Engineering News*. 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 four postdocs, eight graduate students, and several visiting researchers.

Over the past year, Robert Langer received honorary degrees from the Gerstner Graduate School at the Memorial Sloan Kettering Cancer Center; the National Institute of Astrophysics, Optics and Electronics (Mexico); the University of Illinois; the University of Limerick (Ireland); and the University of Laval (Canada). He was presented the Kabiller Prize in Nanoscience and Nanomedicine, the Memorial Sloan Kettering Medal for Outstanding Contributions to Biomedical Research, the American Chemical Society Leadership Award for Historic Scientific Advancement, and the Alpha Omega Dental Fraternity Achievement Medal Award. Professor Langer delivered the Suslick-Sessler Lecture in Materials Chemistry (University of Illinois), the Henry Louis Smith Lecture (Davidson College), the Tetelman Lecture (Yale University), the Stetson Lecture (University of Vermont), the Deloitte Endowed Lecture (Dana-Farber Cancer Institute), the Alfred Stracher Memorial Lecture (SUNY Downstate Medical Center), the Bernal Distinguished Lecture (University of Limerick), and the Anderson Distinguished Lecture (University of Virginia). Also, he was the commencement speaker at the Memorial Sloan Kettering Cancer Center's Gerstner Graduate School. He was inducted into the *Advanced Materials* Hall of Fame, and *Nature Biotechnology* named him 2016's top translational researcher.

In his research, J. Christopher Love applies new bioanalytical processes to profile immune responses in chronic diseases, including multiple sclerosis, cancer, and food allergies. His lab continued to advance a new method for single-cell RNA sequencing in collaboration with Professor Alex Shalek (IMES/Chemistry) that is highly portable and accessible for other research labs working with sparse clinical samples. Also, Love and his group continued to work with leading immunology, medicine, and technology laboratories in the Food Allergy Science Initiative in an effort to understand the basic

biology of food allergies and approaches to improve diagnoses. In addition, the group advanced its biomanufacturing programs with both DARPA and the Gates Foundation to develop approaches to improving access to biopharmaceuticals and vaccines using micro-modular manufacturing systems and integrated designs of molecules and hosts. Professor Love continued serving as a scientific advisor to several groups in biomanufacturing and immunotherapies and on the steering committee for the International Conference on Accelerating Biopharmaceutical Development.

Warren K. Lewis Career Development Professor of Chemical Engineering Karthish Manthiram leads a research group that develops methods by which renewable electricity can be used to drive sustainable chemical synthesis. The group's members (six graduate students, three postdocs, and two undergraduate students) have developed new technologies in the past year to synthesize carbon-neutral fuels and fertilizers using air, water, and carbon dioxide. Professor Manthiram's research is supported by Cenovus Energy, Oprex, J-WAFS, MITEI, the Karl Chang Innovation Fund, and Lincoln Laboratory. Manthiram continues to develop new methods for increasing student engagement in 10.426/626 Electrochemical Energy Systems and 10.302 Heat and Mass Transfer, for which he was presented the C. Michael Mohr Outstanding Undergraduate Teaching Award.

Allan S. Myerson continued his research on fundamental and applied problems in crystallization and pharmaceutical manufacturing. In addition, he continued his work as a principal investigator in the Novartis-MIT Center for Continuous Manufacturing and on the DARPA Pharmacy on Demand project. Professor Myerson serves as an associate editor of the ACS journal *Crystal Growth and Design*. He also serves on the scientific advisory boards of BlueSpark, a company that develops novel flexible batteries, and CONTINUUS Pharmaceuticals.

Bradley D. Olsen was awarded the Dillon Medal by the American Physical Society for research accomplishments in polymer physics. In addition, Olsen delivered the Mellichamp Lecture at Purdue University and the Saville Lecture at Princeton University, both in recognition of his accomplishments as an early-career chemical engineering researcher. Olsen was also honored with an MIT Committed to Caring Award. Olsen's research group continued its work in the areas of bioinspired and biofunctional block copolymers, polymer gels, and protein-based materials for applications in defense, sustainability, and human health. Major accomplishments included the development of self-assembled protein nanostructures that can provide large improvements in biosensing capability, the discovery of new formulations that can improve the processing of proteins into sustainable materials, and the establishment of new methods to understand the mechanisms by which hemostats act so that they can be developed with improved efficacy. In addition to this work, the group is actively engaged in starting a company to translate Olsen's research into the cosmetics industry. During the past year, Olsen served as an instructor for 10.40 Chemical Engineering Thermodynamics (at the graduate level) and 10.00 Molecule Builders, a hands-on course introducing freshmen to molecular sciences.

Kristala L.J. Prather, the Arthur D. Little Professor of Chemical Engineering and a member of the MIT Synthetic Biology Center, continues to focus on microbial synthesis of chemical compounds. Prather serves on several scientific advisory and editorial

boards and is an associate editor of *ACS Synthetic Biology* and *Metabolic Engineering Communications*. Also, she continues her service to the government as a member of the DOE Biological and Environmental Research Advisory Committee and the National Academies of Sciences, Engineering, and Medicine Committee on Strategies for Identifying and Addressing Biodefense Vulnerabilities Posed by Synthetic Biology. This summer marked the end of her two-year term as a member of the World Economic Forum's Global Future Council on Biotechnology. Within MIT, Prather continues to serve as director of the long-running Fermentation Technology course (popularized by Professor Daniel I.C. Wang and offered through MIT Professional Education), as bioengineering systems lead for the MIT-Portugal Program, and as faculty co-director of MITEI's Energy Biosciences Low-Carbon Energy Center. Within the department, Prather chairs the Task Force on the Undergraduate Curriculum, which to date has led the approval of two changes to the degree requirements. This year she concluded a five-year term as co-director of the Microbiology Graduate Program, an interdisciplinary initiative involving faculty from the Schools of Engineering and Science.

Gregory C. Rutledge is the Lammot du Pont Professor of Chemical Engineering. His research group develops molecular simulations for the study of fundamental process-structure-property relationships in polymers, with a particular emphasis on crystallization kinetics and thermomechanical properties of polymers with complex morphologies. This year NSF renewed for another four years his initiative combining computation and experimentation to accelerate the design and discovery of additives for semicrystalline polymers. His group is also active in the development of ultra-fine fibers for various applications in clean air, clean water, and advanced materials. Professor Rutledge continues to serve as the lead PI for Advanced Functional Fabrics of America, and, in collaboration with AFFOA and the Fashion Institute of Technology (FIT), he organized the first FIT/MIT Workshop on Advanced Fibers and Fabrics, which brought together students with diverse interests in design, fashion, engineering, and materials to rethink the clothing of the future. In terms of teaching, Rutledge continues to revise the junior/senior-level 10.26/27/29 Chemical, Energy, and Biological Engineering Projects Lab; this year he initiated the first team competition, culminating in final presentations before the entire department. At the graduate level, he is reinventing the core 10.568 Physical Chemistry of Polymers class. Over the past year, Professor Rutledge delivered invited lectures in Germany, Switzerland, the Netherlands, and the United States. He continues to serve as editor of the *Journal of Materials Science* and on the IUPAC Task Force for Terminology in Modeling and Simulation of Polymers.

Esther and Harold E. Edgerton Career Development Chair Hadley D. Sikes continued to lead her team in using an approach based on engineering design to invent and integrate protein and polymer technologies into point-of-care medical diagnostic tests. This year the team is evaluating, with clinical partners at Brigham and Women's Hospital and the Tufts Medical Center, new and practical analyses of gene-specific promoter methylation and redox metabolism in tumor biopsies to guide selection of effective therapies. In the area of infectious disease, SMART and the Tata Center have facilitated field analyses in Southeast Asia of rapid paper-based tests of urine for proteins that indicate tuberculosis and blood for proteins that indicate malaria. Sikes is a PI in SMART's new IRG focused on combating antimicrobial resistance. She delivered seminars at Princeton, Berkeley, and Stanford and invited talks at meetings of EMBO, AIChE, and ACS. In partnership

with AIChE's Society for Biological Engineering, Professor Sikes launched the first International Conference on Epigenetics and Bioengineering and served as its chair. Also, she is contributing to the launch of the new journal *ACS Applied Bio Materials* by serving on its first editorial board. Sikes was honored by the National Academy of Engineering as an innovative young engineer and by MIT graduate students as a recipient of the Committed to Caring Award.

Zachary P. Smith joined the Department of Chemical Engineering in January 2017 and currently holds the Joseph R. Mares Career Development Chair. His research focuses on the development of polymers and porous materials for applications in energy-efficient separations. In 2018, Professor Smith and his research group received several awards. Most notably, Professor Smith was selected to receive the Department of Energy Early Career Award. This award, which comes with five years of research support, is designed to bolster the nation's scientific workforce by providing career recognition and support to exceptional researchers during the crucial early career years, when many scientists do their most formative work. Professor Smith also was presented the ACS Petroleum Research Fund Doctoral New Investigator Award and received funding from J-WAFS to develop new boron removal technologies for water purification. In May 2018, Professor Smith's visiting student Francesco Benedetti, who served as the co-founder and president of the MIT Visiting Student Association, won two Institute awards: the Golden Beaver Award and the William L. Steward, Jr. Award. Additionally, Professor Smith's student Albert Wu received the NSF Graduate Research Fellowship Award. Professor Smith taught 10.569 Synthesis of Polymers in the spring term and will teach 10.467 Polymer Science Lab this fall. He currently advises five graduate students, two postdoctoral scholars, a visiting researcher, and two undergraduate students.

George Stephanopoulos stepped down from his full-time professorship and retired from MIT. An international two-day symposium titled 2040 Visions of Process Systems Engineering was organized at MIT in June 2017 to celebrate Professor Stephanopoulos's 70th birthday and his many contributions to process systems engineering education and research at MIT and beyond. With more than 200 participants, the symposium included presentations and discussions on the future of process systems engineering, as well as a reunion of former and current students, postdocs, and colleagues of Stephanopoulos. By all accounts, the symposium was a very successful event. In September and October 2017, the University of Kyoto invited Professor Stephanopoulos as a distinguished visiting professor; while there, he gave a series of lectures on advanced subjects such as the foundations and historical evolution of process systems engineering, systems thinking in the management of process operations, and game-theoretical approaches to multi-actor distributed processing.

Gregory Stephanopoulos, the W.H. Professor of Biotechnology and Chemical Engineering, completed another year as director of the Metabolic Engineering Laboratory. In this capacity, he supervises the work of 25 to 30 researchers who focus on engineering microbes to convert them to little chemical factories for the production of fuels and chemicals. Notable research successes this year included the engineering of an oleaginous yeast to achieve record levels of lipid accumulation and advancement of an integrated system for the fixation of CO_2 into acetate. These developments contributed to replacement of fossil feedstocks and advancement of the vision of a biobased

economy. In parallel, he continued to investigate the metabolic aspects of cancer, with a particular focus on the identification of metabolic targets. Professor Stephanopoulos serves on the advisory boards of four academic institutions, is the past president of the American Institute of Chemical Engineers, and is a member of the managing board of the Society for Biological Engineering. He delivered the 2017 Kroc Memorial Lecture at the University of Chicago. During the past year, he continued to serve as editor-in-chief of *Metabolic Engineering* and *Current Opinion in Biotechnology* and on the editorial boards of eight other scientific journals. In addition to numerous research presentations at professional society meetings, he delivered plenary and keynote lectures at the International Conference on Metabolic Science, the Metabolic Engineering Summit, and the Biochemical Horizons Symposium. Also, he was honored with the Novozymes Award for Excellence in Biochemical and Chemical Engineering.

Michael S. Strano was inducted into the National Academy of Engineers in October 2017. He has continued his research into nanotechnology and low-dimensional materials, addressing problems in energy, plant biotechnology and agriculture, and medical devices. He was awarded a Professor Amar G. Bose Research Grant for the development of a nanobionic light-emitting plant and published the first prototype in the journal *Nano Letters*. Also, his laboratory invented the first completely synthetic, cellular-sized autonomous electronic devices capable of collecting and processing information from exotic environments; details on these devices, called colloidal state machines, were published in *Nature Nanotechnology*. In addition, Strano and his laboratory invented new energy-harvesting devices called thermal resonators, which generate electrical power from thermal oscillations that are ubiquitous in the environment. Prototype devices are being tested on the roof of Building 66, and his students are generating a start-up, Ecto-Therm, already the recipient of several business development awards. Professors Strano and Jacopo Buongiorno (Nuclear Science and Engineering) invented a new low-temperature wetsuit for arctic temperature diving by modifying the material neoprene, addressing a long-standing problem presented to them by the US Navy SEALs. Strano continues his editorial duties for the journals *Carbon* and *Current Protocols in Chemical Biology*.

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. His work was featured in eight peer-reviewed publications; one study published in *Physical Review Fluids* described the development of new models for the settling of colloidal dispersions that can be readily applied in environmental and pharmaceutical sciences. The Swan group currently has six graduate students and three undergraduates and hosted several international students in the spring and fall.

William A. Tisdale, the ARCO Career Development Chair in Energy Studies, leads an experimental research team investigating the synthesis and photophysical properties of colloidal semiconductor nanocrystals for use in next-generation energy technologies. Professor Tisdale is particularly dedicated to undergraduate education, having twice received the departmental undergraduate teaching award as well as the Institute-wide Baker Award for Excellence in Undergraduate Teaching. Over the past year, Tisdale has

been a driving force behind the department's undergraduate curriculum revitalization effort, and beginning in 2018 he will serve as the faculty advisor for the Baker Foundation Advisory Committee.

Bernhardt L. Trout continues in his role as director of the Novartis-MIT Center for Continuous Manufacturing, an $85 million partnership that just finished its second successful phase. In addition, he is director of the Society, Engineering, and Ethics (SEE) program, which held courses for 140 students this past year. This program enhances the breadth and depth of engineering students' knowledge, teaching them the connections between engineering and society. His laboratory focuses on pharmaceutical small-molecule manufacturing and biopharmaceutical formulation and stabilization, including predictive methods that are used by pharmaceutical companies around the world. He is a consultant to the FDA and co-chair of the International Symposium on Continuous Manufacturing of Pharmaceuticals. In addition, he is on the scientific advisory boards of a number of major companies and is involved in several start-up companies. Over the past year, Professor Trout delivered many invited talks along with publishing research papers and submitting patents.

Research Highlights

Electrochemically Modulated Processes for Chemical and Environmental Separations (T. Alan Hatton)

Water scarcity, both economic and physical, affects close to a third of the world population. Efficient, affordable, and robust purification technologies are needed for a range of separation contexts, from point-of-source treatment or remote in situ purification devices to large-scale, centralized wastewater treatment facilities. Micropollutants (e.g., organic endocrine disruptors, pesticides, household chemicals, dyes, and heavy metal cations) are a particularly vexing problem in wastewater treatment, since current technologies suffer from high energetic penalties and performance limitations when confronted with pollutants at very low concentrations, often in the presence of excess competing species. Similarly, the increased use of heavy metals and metalloids in industrial, agricultural, and technological applications has led to their wide distribution and persistence in natural water bodies and soil; elements such as lead, cadmium, nickel, mercury, arsenic, and copper may cause multiple organ damage even at low exposure levels, and thus they are of public health significance. The production of metals through extraction and refining generally results in process streams containing diluted metals that are discarded with the tailings to sedimentation ponds, but there is now strong interest in exploring the potential for economical recovery of such metals from waste streams.

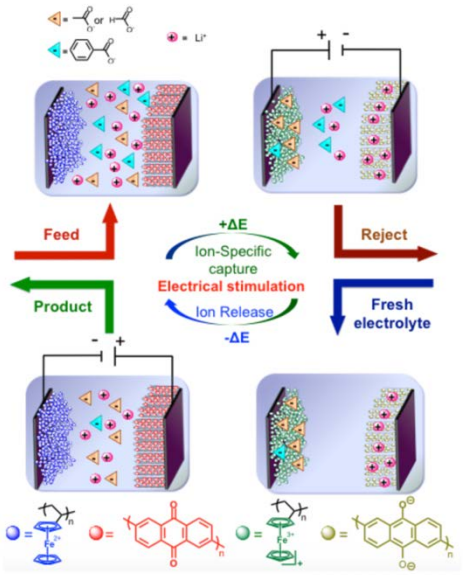

Figure 1. Redox-activated electro-swing adsorption technology concept.

To address these concerns, we have developed a platform purification technology based on redox-mediated electrochemical modulation of the separation environment, which can, in many cases, offer significant advantages over conventional separation methods (the concept is illustrated in Figure 1). Redox-mediated chemical moieties tethered to electrode surfaces can be tailored to ensure adsorptive selectivity with high separation factors toward toxic pollutants in one oxidation state and release of these compounds when the oxidation state is changed; this sorption swing can be achieved with low overpotentials and high current efficiencies. We exploit organometallic polymeric electrodes to target pollutants ranging from pesticides to toxic heavy metals. Capture and release are controlled solely by the electrochemical potential, and thus there is no need for chemical regenerants or post-treatment; also, there is little chemical waste, and water usage ratios are low. In addition, an asymmetric configuration can be implemented to achieve higher levels of electrochemical performance and energy storage; at the same time, we control the water chemistry and thus enhance separation factors. Finally, through materials optimization, we have shown the strong stability of these electrodes for more than 500 cycles with over 95% current efficiency. Significantly lower energy consumption is observed (estimated to be approximately 0.3 to 1.0 kWh/m^3 purified water) than with traditional methods, which results in a reduced carbon footprint. In addition, due to their electrochemical nature, redox-based systems can be easily integrated with renewable energy sources in remote locations (e.g., agricultural waterscapes or villages in the developing world). In the long term, energy-efficient selective electrochemical methods offer a powerful solution for water purification and resource recovery across a range of scales. Figure 2 shows some of the results obtained for removal of organic anions from a large excess of salts in solution and removal of toxic hexavalent chromium from dilute aqueous solutions.

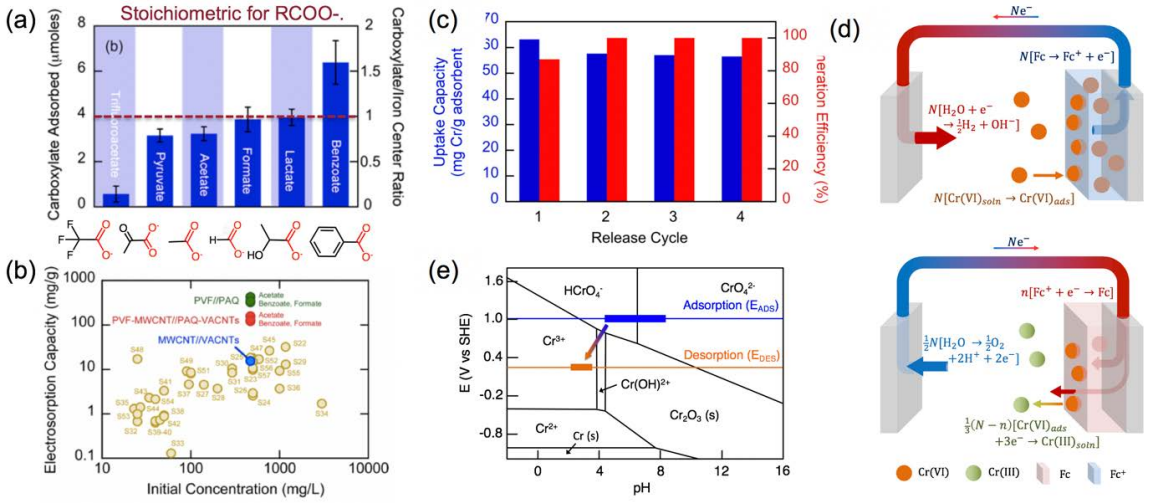

Figure 2. (a) Carboxylic anions interact selectively and stoichiometrically with ferrocenium moieties in a 30-fold excess of competing anions. (b) The electrosorption capacity of the redox systems is significantly greater than that of conventional capacitive deionization systems. (c) Cyclic stability in the capture and release of hexavalent chromium. (d) Schematic of sorption of Cr(VI) and desorption of Cr(III) during electro-swing operations. (e) Pourbaix diagram showing speciation changes during adsorption and desorption of chromium species.

CO_2 Mitigation

The capture of anthropogenic carbon dioxide from industrial and power generation sources, where the concentration of CO_2 is relatively high, is an important component

in an overall portfolio of low-carbon energy sources for climate change mitigation. The US Department of Energy acknowledges, for instance, that for the foreseeable future coal, oil, and natural gas will continue to play a critical role in national and global electricity generation and that innovations in the field of carbon capture from high concentration sources such as fossil fuel combustion and gasification units are crucial. In addition, on-board carbon capture for reduced emissions from vehicles and other mobile sources, which account for almost 30% of all emissions in the United States, has garnered interest over the last few years from the automotive and gas and oil industries. Other sources of much lower CO_2 concentrations collectively represent a large volume of carbon emissions, and there is thus a growing interest on the part of DOE and private industries in capture technologies that operate over a wide range of CO_2 concentrations, especially concentrations below 1%. There is also a significant benefit to innovations in removal of CO_2 from enclosed spaces, such as those in buildings, aircraft, spacecraft, and submarines, where the concentration of CO_2 is in the 1,000 to 10,000 ppm (parts per million) range and the small spaces available limit the types of capture technologies that can be used. Removal of CO_2 from buildings to reduce its overall concentration to levels acceptable for human activity will limit the need for frequent air exchanges and thereby reduce energy needs for conditioning of fresh air brought into the buildings; this in turn results in fewer CO_2 emissions from power plants.

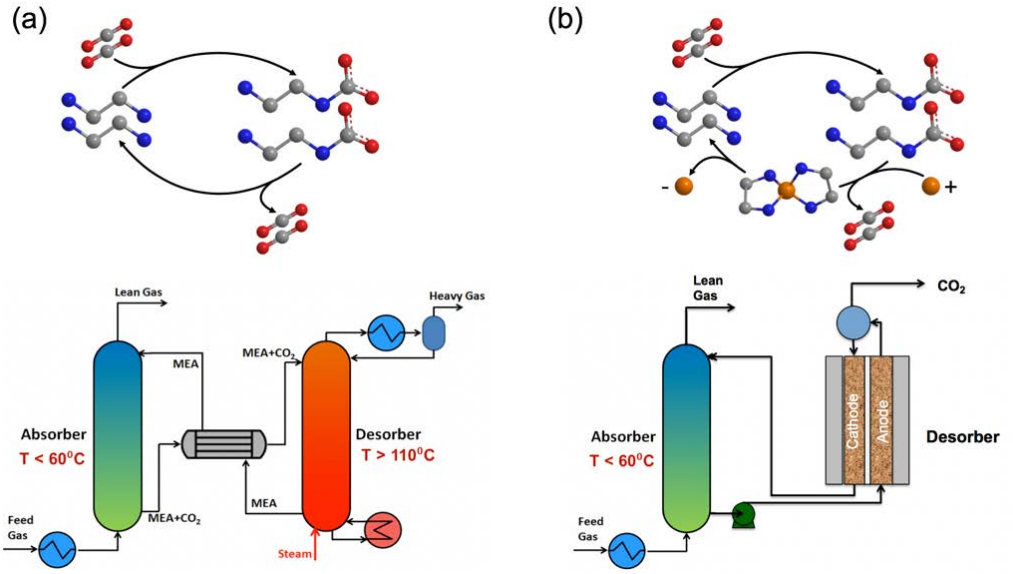

Figure 3. (a) Conventional amine sorption temperature-swing operation with desorption through heating. (b) EMAR system in which Cu^{2+} from oxidation of the copper anode displaces and releases the CO_2; the amine is regenerated on plating out of the copper in the cathode chamber.

The state-of-the-art technology for carbon capture from a flue gas source is the thermally regenerated amine process. This process still faces challenges that have slowed down its rapid deployment at very large scales. Among others, these challenges include high-temperature degradation of amines, the high costs of retrofitting existing power and chemical plants, and the high operational costs associated with carbon capture. Continued efforts have been made to address these challenges on many fronts. Our group at MIT has proposed an electrochemically mediated amine regeneration (EMAR) process that can operate at temperatures under 60°C. A simplified EMAR process flow diagram is shown in Figure 3. Initially, the CO_2 bound amine (e.g., ethylenediamine [EDA]) is sent to the anodic

compartment of an electrochemical cell. The metallic (e.g., Cu) electrode dissolves under electrical polarization to release metallic cations into the solution. The stability constant for the Cu-EDA complex is much larger than that for the EDA-carbamate complex, with the result that CO_2 is desorbed from the aqueous amine solution. In the cathodic compartment of the electrochemical cell, metallic Cu is plated out from the aqueous solution, thereby regenerating the amine for further capture of CO_2 in the absorber. A background electrolyte (e.g., $NaNO_3$) is used to minimize resistive losses in the electrochemical cell. The EMAR process involves several major advantages: (1) it can be operated at low temperatures, thereby minimizing amine degradation; (2) it operates mainly on electrical energy, and thus retrofitting may be more cost effective because there is no need for any (or significant) modification to the existing steam cycle; (3) it offers the possibility of desorbing CO_2 at moderate pressures, thereby minimizing downstream compression costs related to CO_2 storage; and (4) the modular nature of electrochemical cells allows for easier scale up and operation with fluctuating loadings. Work is currently underway to scale this process for installation in an IHI pilot facility in Japan.

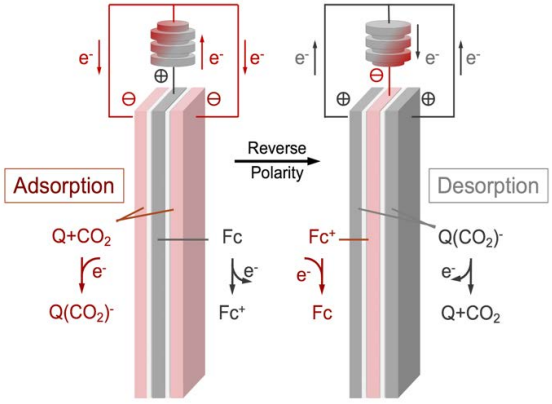

Figure 4. Electro-swing process for CO_2 capture and release. During adsorption, quinone moieties are reduced and complex with CO_2; the center ferrocene electrode is a source for the electrons. On reversal of the potential, the oxidized quinones release the CO_2, and the ferrocenium moieties are reduced back to the neutral ferrocene.

In another approach to CO_2 capture, we have developed asymmetric supercapacitor assemblies with novel architectures (shown in Figure 4) for the electrosorption and subsequent release of carbon dioxide over a wide range of feed concentrations. The electrodes rely on Faradaic pseudocapacitance in which gas uptake and release are regulated by changes in the redox state of a functional group. We have successfully developed facile methods for the preparation of the electrodes, including their chemical synthesis and assembly into the working cell; the electrochemical characterization of the electrode assembly; and the dynamic uptake and release of the targeted compounds under a range of different operating conditions, including both batch and cyclic continuous flow systems. Experimental results from a bench-scale prototype show up to 80% capture of CO_2 from inlet streams of CO_2 concentrations as low as 0.5% (5,000 ppm) at a Faradaic efficiency above 70%. In a three-way industrial collaboration (MIT, Eni, and FCA), we are currently working to install a prototype unit on board a vehicle.

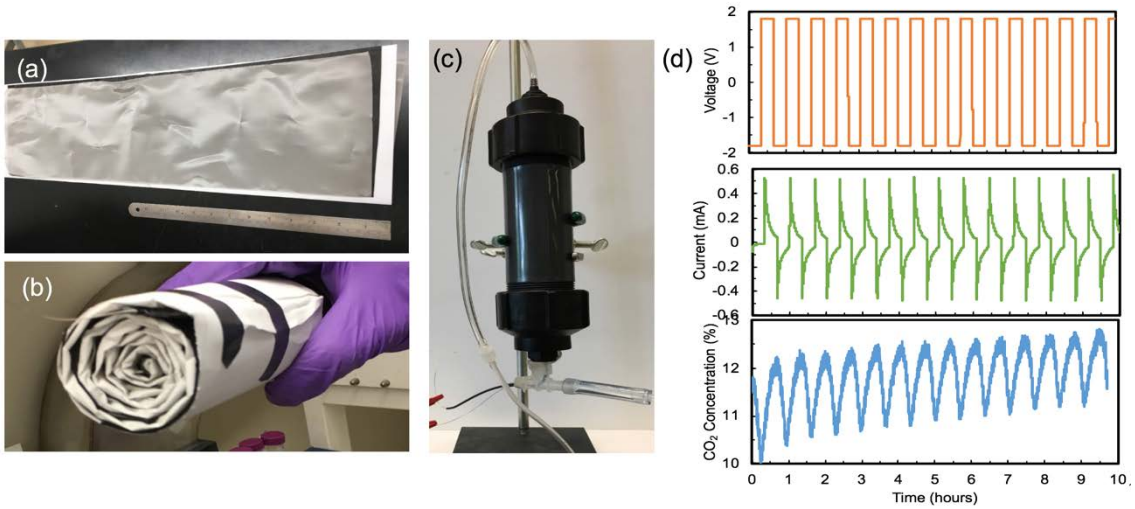

Figure 5. (a) The electrode sandwich. (b) The rolled electrode for insertion in a column. (c) The assembled module for CO_2 capture. (d) Experimental results showing current variations and outlet CO_2 concentrations as modulated by the applied voltage.

Accelerating Inorganic Discovery with Machine Learning and Automation (Heather J. Kulik)

In recent years, tremendous advances in computing power have transformed everyday life. These same advances have made it increasingly possible to carry out complex scientific computations involving large, intricate systems with high fidelity. Despite current efforts that have directed computation toward the discovery of new materials, scientists have explored very little of the vast chemical space (as little as one part in 10^{50}) that could contain as-yet-unknown molecules and materials with desirable properties. Transition metal complexes consisting of an open-shell metal surrounded by organic matter that tailors the metal's local electronic properties are widely employed as sensors, in lighting, and for energy storage. The same highly tunable electronic structure properties of transition metal complexes that make them attractive for application as functional materials or catalysts make exploration of their "neighborhood" in chemical space daunting. Here discovery efforts are hampered by the combined challenge of the dimensionality (e.g., variable coordination of metals with ligands) of chemical space and the complexity of structure-property relationships, which necessitates direct experimental or quantum mechanical characterizations. Although advances in computing power have made quantum mechanical calculations via density functional theory (DFT) increasingly routine for materials characterization, DFT in practice is simultaneously too inaccurate and too inefficient for the predictive transition metal chemical space exploration needed to discover new molecules and materials. Our research program has addressed these challenges by bridging accelerated first-principles simulation with new data-driven and machine learning concepts. We have built and demonstrated an integrated open-source software platform for automating inorganic catalyst and materials design that dramatically overhauls computational chemistry studies from initial structure generation to accelerated structure-property relationship determination using machine learning. We simultaneously advance understanding of DFT accuracy and improve DFT methodology to support our discovery efforts.

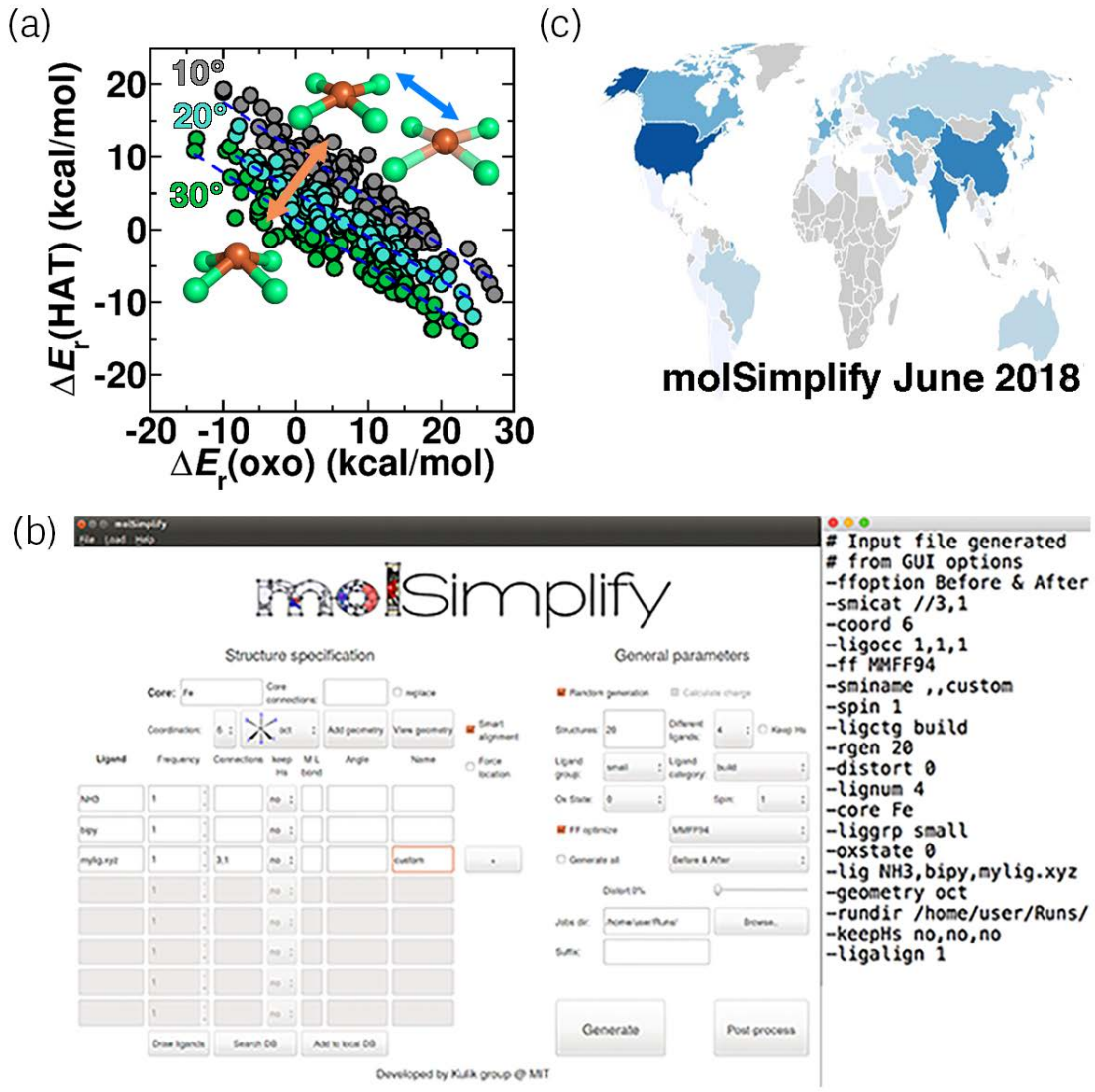

Figure 6. (a) Hydrogen atom transfer (HAT) versus oxo formation (oxo) reaction energies across a catalyst test set; the changing metal-ligand plane angle shifts and disrupts scaling relations. (b) molSimplify graphical interface. (c) molSimplify usage in June 2018 (increasing from light blue to dark blue; gray signifies no usage).

We have developed the first open-source toolkit for inorganic discovery with the long-term goal of making the twin challenge of complexity and dimensionality in transition metal chemical spaces tractable for any design objective (Figure 6). Since its introduction in 2016, our molSimplify toolkit has seen increasingly wide use. The toolkit and its recent extensions for periodic systems tackle the following key challenges related to computational materials discovery: generation of high-quality structures, acceleration of first-principles simulation and characterization, and automated determination of structure-property relationships for optimum catalyst or material identification, including iterative chemical space searching. Our divide-and-conquer approach harnesses informatics tools that have long guided chemical discovery in organic chemistry and extends them through quantum-mechanical design rules where organic chemistry principles would prove insufficient. A unique feature of our toolkit is the rapid, unbiased generation of new catalysts and materials from multimillion-molecule databases of previously experimentally synthesized building blocks to ensure realism in

computational discovery. We have applied these tools to several challenges ranging from catalyst and materials design to materials synthesis.

Our screening methodology enables us to uncover paradoxical results and design principles that defy conventional chemical intuition and rules. Conventionally, optimization of heterogeneous catalysts relies on chemical rules encapsulated in so-called linear free-energy relationships (LFERs); relative free energies of similar intermediates are thought to be closely related to each other, enabling simplified screening of a complex reaction mechanism involving dozens of intermediates and transition states. However, LFERs also reveal a fundamental limitation in heterogeneous catalyst optimization: typically improving the kinetics associated with one step of a reaction worsens others, producing a limitation in the maximum selectivity or activity of a catalyst. We have used our molSimplify discovery toolkit to identify limits and exceptions to LFERs in more variable, readily tailored single-site catalysts. In an automated, high-throughput study of over 540 catalyst variations, we found that metal-ligand plane distortion in single-site catalysis offered an opportunity to overcome the conventional limitations of volcano-type (i.e., narrow and peaked) activity for the challenging but valuable process of direct conversion of methane to methanol. We have employed these same tools to discover exceptions in design rules for building blocks used in quantum dot synthesis, CO_2 sequestration catalysts, and redox couple designs for energy storage.

Automating first-principles discovery has led to a number of valuable insights; to address multifaceted optimization challenges, however, there is a need to develop faster-than-DFT routes to property prediction in inorganic chemistry. We have developed the first machine learning models (here an artificial neural network [ANN]) for predicting quantum mechanical properties of transition metal complexes. Using these advances, we have predicted DFT bond lengths and spin-state or redox energetics at near-chemical accuracy and DFT model sensitivity in seconds rather than hours.

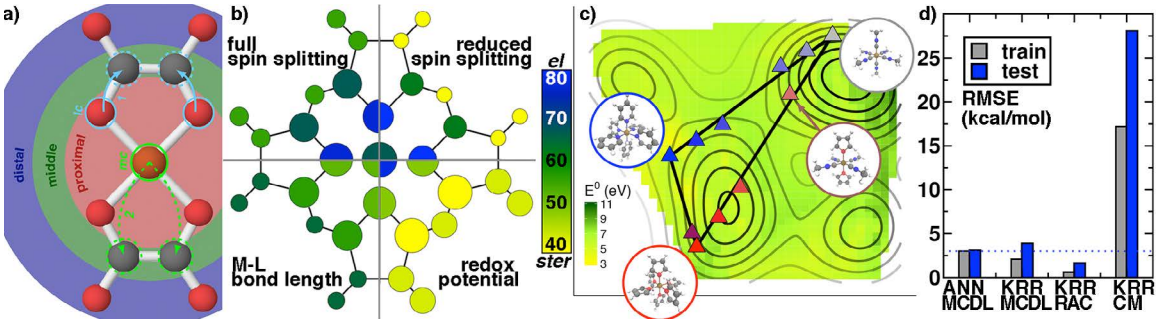

Figure 7. (a) Schematic of developed descriptors that enable (b) structure-property determination, wherein the relative balance of electronic (el, blue) and steric (ster, yellow) properties is indicated on a porphyrin molecular graph for two spin-splitting sets (full versus reduced), metal-ligand (M-L) bond length prediction, and redox potential prediction. (c) A map of complexes with data density indicated by contours in the redox potential descriptor set revealing complex similarity relationships. (d) Performance of our models (MCDL or RAC) versus prior work (CM) with neural networks (ANN) and kernel ridge regression (KRR) on training set and unseen test set molecules.

Expanding upon the first representations we developed (mixed continuous and discrete local descriptors [MCDLs]), we have introduced adaptive, topological descriptors

tailored for inorganic chemistry that outperform prior efforts in machine learning that have focused only on organic bonding (RAC [revised autocorrelation function] or MCDL versus prior work [KRR/CM] in Figure 7). When combined with feature selection tools, our new descriptors (RACs, demonstrated in Figure 7a) reveal the length scales of essential structure-property relationships (Figure 7b). This approach automates the discovery of structure-property relationships to reveal design rules in inorganic chemistry and identify opportunities for orthogonal, multi-objective design (Figure 7b). For example, abstraction on the kilo-compound scale of essential drivers of spin splitting and redox potential reveals that the former is much more sensitive to metal-local electronic properties, whereas the latter is sterically driven and non-local, suggesting that the two properties could be tuned independently (Figure 7b). These representations also map out transition metal chemical space, suitably describing how similar or dissimilar complexes are to enable accelerated design (Figure 7c). Our representations preserve desirable traits for application to experimental data sets. We have received support from DARPA to apply our representations for machine learning of large metal-organic frameworks from literature data sets in order to guide simulations in our lab and experimental efforts in Zachary Smith's lab.

Beyond property prediction alone, our primary objective is to accelerate discovery of new materials. We have incorporated evolutionary algorithm–driven optimization with these machine learning models for accelerating high-throughput screening with knowledge of model uncertainty. From a large compound space, we discovered new spin crossover (SCO) functional materials. SCOs consist of open shell metals with near-degenerate spin states (i.e., electronic states that differ in the number of paired electrons) that change in response to light or temperature, making them ideal materials for spintronics and sensing. Of these thousands of compounds, only 2% had been seen via our machine learning model, and replacing DFT evaluation with machine learning evaluation provided orders of magnitude speedup (Figure 8).

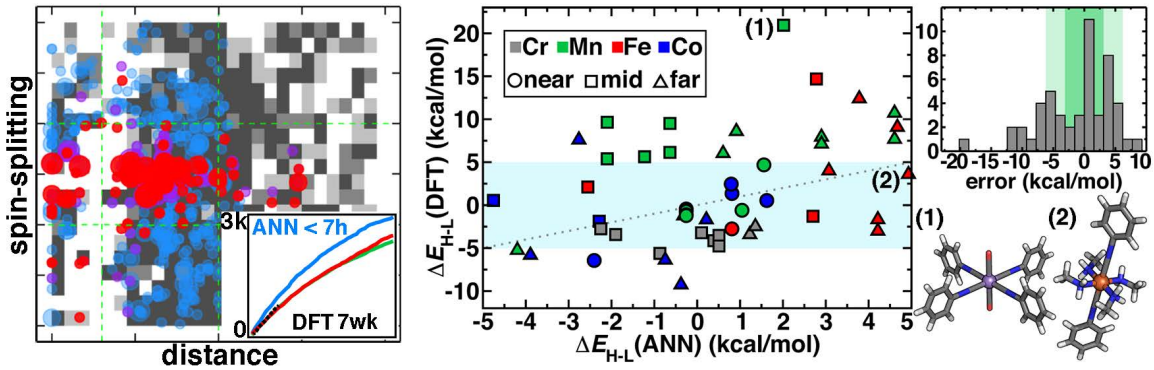

Figure 8. (left) Schematic of evolutionary algorithm (EA) exploration of a large (>5,500) compound space, with points sampled indicated at the beginning of the EA run by blue dots, then purple, then red (as indicated in the inset color bar); the size of the dot corresponds to how frequently the structure was retained. The inset shows how many of the compounds are sampled by the EA and the time of an ANN versus full DFT calculation. The axes correspond to the spin-splitting and the distance to training data, with the target region indicated by the two sets of green dashed lines. (middle) Subset of 50 complexes selected as SCOs by ANN and validated DFT energetics. Two thirds of compounds remain SCOs (inside the blue region) after full validation. (right, top) Error histogram of ANN errors with respect to DFT validation, with the inner green region showing 1x baseline error (40% of points) and the outer region showing 2x baseline error (80% of points). (right, bottom) Example corresponding to the middle pane of a high-error, mid-distance Mn-complex point (1) and a validated SCO with low error but a high-distance Fe-complex point (2).

Once leads were discovered through evolutionary algorithm optimization, we validated them via DFT to determine whether they were true SCOs (Figure 8). Although the tight energetic criteria for an SCO (within 5 kcal/mol) were close to the baseline error of our ANN model, more than two thirds of these new complexes were confirmed SCOs, and most ANN errors were within 2x test error of the ANN on previously seen complexes (Figure 8). This approach enabled discovery of unconventional SCOs, including those that mixed strong and weaker field ligands not expected on the basis of conventional inorganic chemistry intuition ((2) in Figure 8). It also highlighted cases in which new chemistry, previously unseen via our ANN, led to unexpected non-SCO behavior ((1) in Figure 8). These divergences highlight the opportunity to develop expected-improvement-based optimization schemes where, instead of avoiding low-certainty, high-promise predictions, algorithms exploit these regions of chemical space to accelerate discovery. We are actively developing such algorithms as well as multi-level modeling workflows for discovery of new inorganic materials, including SCOs, redox couples in redox flow batteries, and metal-organic frameworks.

Our work in accelerating inorganic discovery through machine learning and automation has benefited from the generous support of the Department of Energy, the National Science Foundation, and the Department of Defense, most recently through a 2018 DARPA Young Faculty Award and a 2018 Office of Naval Research Young Investigator Award. This multidisciplinary chemistry and materials research has been recognized in a number of ways, including through the ACS OpenEye Outstanding Junior Faculty Award in Computational Chemistry and upcoming featured talks at the ACS "Artificial Intelligence & Its Impact on the Chemical Enterprise" symposium and the Caltech Resnick Young Investigators Symposium. The Kulik group's efforts have been highlighted in press pieces and journal virtual issues, including a feature in *Chemical & Engineering News.* In addition, their work has been summarized in a number of invited articles, including an article for a special issue of *Industrial & Engineering Chemistry Research* and an upcoming "Rising Stars" piece for *Frontiers in Chemistry*. This year, the Kulik lab has established funding for cross-disciplinary efforts with experimentalists in catalysis and materials synthesis both at MIT and beyond to apply Kulik's machine learning and automation tools to guide experimentally validated transition metal chemical space exploration. These extensions are expected to dramatically reduce the time to discovery of new materials and catalysts, enabling rapid exploration of vast and as-yet-unknown regions of transition metal chemical space.

Annual Lectures and Seminars

During 2017–2018, the Chemical Engineering Department hosted a distinguished group of academic and industry leaders speaking on topics highlighting cutting-edge research that addresses today's energy and health-related challenges. Webcasts for all major lectures can be accessed on the department's website.

15th Daniel I.C. Wang Lecture on the Frontiers of Biotechnology (September 8, 2017): "The Future of Drug Discovery: Innovation-Driven Research & Development at Takeda." Andrew Plump, chief medical and scientific officer at Takeda Pharmaceuticals International, discussed his work, including leading Takeda's global research and development (R&D) organization. To continue to accelerate Takeda's R&D successes,

he leads a team that focuses on people and partnerships, modality diversification, translational medicine, and genomics. Prior to assuming his current role, Plump served as senior vice president of research and translational medicine and deputy to the president of R&D at Sanofi, where he was responsible for global research and translational medicine across all therapeutic areas.

32nd Hoyt C. Hottel Lecture (December 8, 2017): "The Clean Energy Transformation." Ernie Moniz, Cecil and Ida Green Professor of Physics and Engineering Systems (emeritus) and special advisor to the MIT president, presented his thoughts on today's clean energy challenges. Moniz served as the 13th United States secretary of energy from 2013 to January 2017. As secretary, he advanced energy technology innovation, nuclear security and strategic stability, cutting-edge capabilities for the American scientific research community, and environmental stewardship. He placed energy science and technology innovation at the center of the global response to climate change and negotiated the Iran nuclear agreement alongside the secretary of state. Moniz joined the MIT faculty in 1973 and was founding director of the MIT Energy Initiative.

24th Alan S. Michaels Lecture (April 6, 2018): "SmartInsulin: A Journey from Course X to Biotech Startup to Big Pharma." Todd Zion, president and CEO of Akston Biosciences, discussed his work, including the development of an injectable therapy for antigen-specific prevention of type 1 diabetes. Prior to starting Akston Biosciences, Zion founded SmartCells Inc. to develop SmartInsulin, the first glucose-regulated injectable formulation for treating diabetes. As SmartCells's president and CEO, Zion was instrumental in raising $10 million in financing from individual investors and another $10 million in grants to support research and clinical development.

40th Warren K. Lewis Lecture (March 9, 2018): "Reinterpreting the Genetic Code." David Tirrell, provost and Ross McCollum-William H. Corcoran Professor of Chemistry and Chemical Engineering at the California Institute of Technology, lectured on his current research. Tirrell was educated at MIT, where he did undergraduate research with Ed Merrill, and at the University of Massachusetts Amherst, where he earned his PhD under the supervision of Otto Vogl. His research interests reside in macromolecular chemistry and the use of non-canonical amino acids to engineer and probe protein behavior. His contributions to these fields have been recognized by his election to the American Academy of Arts and Sciences and to all three branches (Sciences, Engineering, and Medicine) of the US National Academies.

Departmental Awards

The department's awards ceremony took place on May 14, 2018, in the Gilliland Auditorium of the Ralph Landau Building. We are pleased to recognize this year's recipients of the Outstanding Faculty Awards: James Swan was the graduate students' choice, and Karthish Manthiram was selected by the undergraduate students.

The Edward W. Merrill Outstanding Teaching Assistant Award was presented to graduate student Krishna Shrinivas for his work in 10.302 Transport Processes during the fall 2017 term. PhD student Zongyu Gu won the Outstanding Graduate Teaching Assistant Award for his work in 10.50 Analysis of Transport Phenomena during the fall

term. 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 Justin Swaney and Connor Coley.

Chemical Engineering Special Service Awards were conferred to the members of the Graduate Student Council: Andy Maloney, Cache Hamilton, Caroline Nielsen, Cynthia Ni, Katharine Greco, Kindle Williams, Mickey Stone, Nathan Corbin, Neil Dalvie, Pedro de Souza, Sam Faucher, Sharon Lin, Stephanie Kong, and Webster Guan. Members of the Graduate Student Advisory Board were also recognized: Kindle Williams, Andy Maloney, Sarah Shapiro, Connor Coley, Herman Alberto Parada Hernandez, Zsigmond Varga, Kristen Severson, McClain Leonard, Kimberly Dinh, and Andrew Fiore. In addition, awards were given to the following members of the REFS (Resources for Easing Friction and Stress) group: Neil Dalvie, Garrett Dowdy, Michael Lee, Sakul Ratanalert, Natasha Seelam, and Lisa Volpatti. Neil Dalvie won the Chemical Engineering Rock Award for his contributions to athletic achievement within the department. The following undergraduate students were recognized for their service to the student chapter of AIChE: Michelle Huang, Linh Nguyen, Brian Zhong, Rafid Mollah, Amy Wang, Marjorie Buss, Andrew Blankenship, Morgan Matranga, Natalie Delumpa-Alexander, Erika Ding, Zach Schmitz, Luis Sandoval, Sarah Coleman, Emily Yan, Nancy Wang, and Anjolaoluwa Fayemi.

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 Caspar Stinn. 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 Marjorie Buss. The Wing and Lourdes Fong Prize, awarded to a chemical engineering senior of Chinese descent with the highest cumulative GPA, went to Brian Zhong. The 2018 Phi Beta Kappa inductees were Nina Anwar, Andrew Blankenship, Marjorie Buss, Nicholas Morgante, Jose Rios, Puwanat Sangkhapreecha, and Brian Zhong.

We are pleased to recognize Jean Belbin as the department's Outstanding Employee of the Year for her dedication and exceptional service to faculty, staff, and students. Chemical Engineering Individual Accomplishments Awards were presented to Orpheus Chatzivasileiou, Kristen Severson, Justin Swaney, Sarah Coleman, Catherine Gauthier, Liona Delva, and Jess Cohen-Tanugi. Tricia Campbell received the School of Engineering's Infinite Mile Award.

The Department of Chemical Engineering at MIT has had a very fruitful and rewarding year and is poised for even greater success in the upcoming year.

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

Martin Z. Bazant
Executive Officer
E.G. Roos (1944) Professor of Chemical Engineering