Department of Materials Science and Engineering

It is hard to imagine that any year could be more eventful. The Department of Materials Science and Engineering (DMSE) has rallied in response to the COVID-19 crisis and has come together to examine our culture in response to the national dialogues on race and equity. Danae and Vasilis Salapatas Professor of Metallurgy Christopher A. Schuh stepped down as department head, and Morton and Claire Goulder and Family Professor in Environmental Systems Jeffrey C. Grossman accepted the position, effective January 1, 2020. We are grateful to Professor Schuh for more than eight years of leadership and for the hard work that has led to several new faculty hires, renovated facilities, an increase in endowed funding for faculty chairs and fellowships, and a rebuilt administrative structure. This work has given DMSE a good foundation for the challenges we are currently facing.

As MIT started to react to news of COVID-19, DMSE's academic office and teaching staff launched efforts to support faculty and staff in remote teaching. The administrative and support staff set up home offices where they could continue to perform all of the essential functions that keep the department running. During this time, many members of the community agreed to serve on committees and task forces across the Institute to share their expertise in teaching, finance, personnel issues, and more. To position DMSE for the future, three committees were established to consider spending and staffing in administration, the academic program, and operational activities. To help students transition from campus or local housing, the department set up a response team to provide advice and, in some cases, funding for moving, internet access, and storage; we were able to use the Witt Fund for Undergraduate Assistance for this purpose. Inspired by the care and support the undergraduates offered each other and the compassion they showed for the MIT and DMSE communities, the faculty and department administrations chose to celebrate them with a special award, the Horace A. Lubin Student Resiliency Award of \$100, presented to all of the seniors in the class of 2020.

DMSE participated in ShutDownSTEM with a department-wide forum on June 10. Over 150 members of the community participated in a three-hour Zoom conversation about race and equity in the academic programs, admissions, and faculty hiring. In response to this session and to student feedback, Professor Grossman established weekly office hours for all DMSE community members to continue to voice concerns and to work toward a more equitable and representative future. Resources and notes from these conversations are being gathered for the community to reference.

We are deeply saddened by the death of Professor Emeritus Kenneth C. Russell. Professor Russell was a graduate of the Colorado School of Mines, and he received his PhD from the Carnegie Institute of Technology. He came to MIT in 1964 as an assistant professor, was promoted to associate professor in 1969, received tenure in 1971, and was promoted to full professor in 1978. His research interests were in nucleation theory and radiation damage to materials, and he held a joint appointment in Nuclear Science. Over the course of his career, he held an influential role in our students' lives, serving for many years as chair of both the Departmental Committee on Graduate Students (DCGS) and the Admissions Committee. He retired in 2001 but continued writing, teaching, consulting, and advising in a post-retirement role.

Educational Initiatives

Over the past several years, DMSE faculty have worked with lecturer Jessica Sandland to create online versions of Course 3 subjects, available through MITx and in some cases used in conjunction with the residential degree program. After the campus shut down in March, this resource allowed the undergraduate and graduate degree programs to move to remote learning very quickly. The effort to add further subjects continues.

In the past academic year, DMSE developed and launched an undergraduate curriculum revision, with the first cohort to start the new curriculum in fall 2020. A faculty task force reviewed the entire Course 3 undergraduate curriculum and gathered feedback about program experiences, structure, pacing, and more. The faculty affirmed a vision that the new curriculum will involve through cross-cutting themes that integrate materials classes when appropriate, integrate lab activities and computational thinking throughout the core, and be balanced (in terms of effort) and integrated across our core. Despite the challenges associated with the upcoming academic year, we are excited to launch this new curriculum and look forward to continuous improvement in the coming years.

DMSE has maintained its top position in *U.S. News and World Report's* graduate and undergraduate lists, in the QS World University Rankings by Subject, and in the Shanghai Ranking.

Undergraduate Education

With an incoming sophomore class of 27 students, DMSE's undergraduate enrollment will be 86 students, with approximately 61% women, 31% underrepresented minorities, and 4% international students. Twenty-one students are designated Course 3-A (a flexible degree program often taken by students intending to continue their education in the field of medicine, business, or law). This past academic year, three students graduated with a double major, and two current students are declared double majors.

Graduate Education

The department's graduate enrollment remains strong, numbering 172 in fall 2019. Approximately 29% of graduate students are women and 5% are underrepresented minorities. Twenty-two DMSE students participate in the Program in Polymers and Soft Matter. For AY2021, we anticipate an incoming class of 40, 33% of whom are women.

DCGS presented a preliminary proposal to the faculty about establishing an interdisciplinary PhD program in computational science and engineering wherein the degree would be jointly administered by DMSE and the MIT Center for Computational Science and Engineering. DCGS will continue to gather additional information for the final proposal to be reviewed in AY2021.

Student Organizations

As ambassadors for the department and the field, DMSE's student organizations host events and develop activities for their fellow students and the community. For example, they participate in the Freshman Pre-Orientation Program along with orientation activities and recruiting efforts. In spring 2020, they took an active role in maintaining student connections to MIT and to the department, sending students care packages of snacks and hosting Zoom parties and a trivia night.

The 2020–2021 Society of Undergraduate Materials Scientists officers are president Alby Joseph, vice president Nick Ignacio, career development chairs Lauren Cooper and Thomas Sierra, social chairs Danielle Gray-Steward and Richard Colwell, publicity chair Jeremy Dudo, apparel and commons chairs Jacqueline Ahrens and Jess Arbuckle, outreach chairs and Women/LGBTQ representatives Ella Richards and Ava Waitz, sophomore representative Eyosias Gebremeskel, junior representative Alana Chandler, and senior representative Jeremy Dudo.

The Graduate Materials Council (GMC) officers for 2020–2021 are president Jatin Patil; vice president Sarah Antilla; secretary Haoxue Yan; treasurer Margaret Lee; DCGS representatives Max L'Etoile, George Varnavides, and Kate Reidy; academic chairs Jesse Hinricher, John Ryter, and Sara Sand; social chairs Camille Farruggio, Sunil Mair, Katherine Stoll, and Sonia Zhang; athletics chair Philipp Simons; outreach committee members Jacqueline Baidoo and Somesh Mohapatra; alumni chairs Joshua Kubiak and Leo Zornberg; Graduate Student Council representatives Eesha Khare and Elad Deiss-Yehiely; diversity, equity, and inclusion (DEI) chair Tunahan Aytas; well-being chair Gillian Micale; coffee hour chairs Jaclyn Lunger and Eveline Postelnicu; sustainability chair Ty Christoff-Tempesta; and Materials Research Society Student Chapter president Katherine Mizrahi.

The DMSE Resources for Easing Friction and Stress (REFS) team included Cécile Chazot and Paul Gabrys.

The Women and Gender Minorities of Materials Science (WOMS) officers are Eesha Khare, Eveline Postelnicu, Jaclyn Lunger, Amina Matt, Kate Reidy, and Sara Sand.

GMC was actively involved throughout the academic year on many fronts including DMSE graduate education, student life and well-being, graduate careers, community building, public service, and DEI initiatives. GMC representatives to DCGS organized discussions for student input on curriculum revisions. In addition, GMC organized orientation workshops including a forum to help incoming students find lab groups. During MIT career week, students organized a panel of DMSE alums from industry and law. The well-being chair hosted a meditation workshop. GMC continued Materials Lectures: The Basics, wherein students offered seminars to their peers. The public service chair hosted workshops in coordination with the Priscilla King Gray Public Service Center (PKG Center) that featured topics such as power and positionality, mental health, and homelessness. GMC worked with the DMSE administration to host a virtual visit weekend program for prospective graduate students. The DEI chair hosted roundtables providing graduate students from different identities an opportunity to share their experiences and allow us to identify areas for improvement. Since March 2020, GMC has worked to build community in the department by hosting a DMSE appreciation board; a DMSE weekly challenge on a different topic each week, with winners selected through community voting; and virtual lunches with professors and students discussing topics such as hobbies, pets, careers, and life in general.

REFS created its own set of communication materials to navigate graduate school resources and was part of DMSE's first-year orientation. In addition, the team organized a program in which students were asked what they expected from REFS; the program featured a brainstorming session and a description of REFS conflict-management training. The team also provided confidential support to graduate students in the department during the COVID-19 pandemic through one-on-one support sessions in remote mode.

This past year WOMS launched multiple programs and initiatives including a womxn website, Womxn Office Hours with Professors (to learn about academic paths), the Womxn Journal Club (discussions on topics relevant to women), and Womxn Disclosure (movie viewing). Also, WOMS engaged in efforts to encourage womxn to sign on to the Black Graduate Students at MIT campaign and the RISE (Reject Injustice through Student Empowerment) campaign.

Facilities

Facilities efforts in the spring were largely focused on creating access during COVID-19, working in concert with the department's environmental health and safety representative. Prior to the shutdown, renovations were completed on a lab for Ellen Swallow Richards Professor Frances Ross and a lab for Toyota Assistant Professor Rafael Gomez-Bombarelli.

Fundraising

This past year, DMSE received a generous gift from Thermo-Calc to support the position of professor of the practice in computational materials science and engineering. In December, a gift from Micron Foundation created a faculty research innovation fund to support tenured, mid-career faculty research in electronic materials; funding was awarded to Toyota Professor of Materials Science and Engineering Caroline A. Ross. The Saks Kavanaugh Foundation funded the Kavanaugh Translational Innovation Fellows Program for another year with the hopes of continued future engagement. The Kavanaugh Program is developing a website to reach a larger community and share the fellows' accomplishments.

Personnel

Paul M. Cook Career Development Professor Robert Macfarlane will be promoted to associate professor, effective July 1. His research focuses on the intersection of soft matter, self-assembly, and composite materials design, and he is working to develop design principles for synthesizing new inorganic/organic composite materials wherein nanoscale structures can be manipulated to tune the emergent physical properties of a bulk material. He is an inspiring mentor and outstanding teacher who provides links for his students between the fundamentals of materials chemistry and practical applications in polymers and biomaterials.

Elsa Olivetti will be appointed to an Esther and Harold E. Edgerton Career Development Professorship for a three-year term. This chair is awarded to young faculty members to support new ideas and opportunities in their research.

C. Cem Taşan has been awarded the Thomas B. King Career Development Chair.

Gregory B. Olson joined DMSE as Thermo-Calc Professor of the Practice in January 2020. Professor Olson was educated at MIT, holding an SB, SM, and ScD from our department. Most recently, he held the Walter P. Murphy Chair at Northwestern University. For the next several years, he will spend the spring semester teaching and mentoring DMSE students. His long history of connecting materials computation and design directly to products and industry gives him a unique perspective that will help us amplify our strengths in both computing and entrepreneurship.

Silvija Gradečak joined the faculty of the National University of Singapore in July 2019. She is currently a visiting professor in DMSE.

During the past year, two faculty searches were conducted. For the first search (a DMSEonly search), candidates were sought with expertise and a special interest in the fields of computation, simulation, and theory of materials, especially at the meso scale. This search was successful, and we have identified a finalist and are negotiating the terms of the faculty member's offer. For the other search (a dual search conducted by DMSE and the Institute for Data, Systems, and Society), candidates were sought with proven excellence, vision, and interest in interdisciplinary research in machine learning, data science, and statistics as applied to problems in materials science and engineering. This search was unsuccessful.

DMSE facilities manager Adam Shervanian has left MIT. Kevin Rogers has accepted the position of facilities manager, effective July 1. Kevin has been an MIT employee for several years, most recently as building supervisor for MIT.nano. We are delighted to have his expertise.

Johanna Wilcox has been promoted to financial administrator 2. Johanna joined DMSE in 2018, and her knowledge and innovative approaches have been invaluable to the faculty and staff.

Merton C. Flemings-SMA Professor Eugene Fitzgerald has joined MIT's Quarter Century Club.

Research Highlights

Despite the COVID-19 interruption, DMSE faculty, staff, and students have continued their research in areas of critical societal importance. The interdisciplinary nature of materials science and engineering sparks collaborations inside and outside the department. Three exciting and fruitful collaborations resulted in important publications this year.

John Chipman Associate Professor James LeBeau, Frances Ross, and Assistant Professor Rafael Jaramillo collaborated to establish groundwork for reliable processing of semiconductor technology based on layered (i.e., 2D) materials. Two-dimensional materials have captured the imagination of the scientific community ever since the pioneering work on graphene in the 2000s. However, despite more than 15 years of continuous and worldwide research, there have been no commercial breakthroughs in semiconductor technologies based on 2D materials, in large part due to the difficulty of making the materials reliably and over large areas (e.g., semiconductor wafers). In a pair of publications in the *Journal of Vacuum Science & Technology* and *Advanced Functional Materials*, the MIT research group reported new processes and chemical guidelines for making wafer-scale thin films of 2D MoS_2 and TiS_2 at temperatures sufficiently low to allow for integration into complementary metal-oxide-semiconductor device manufacturing. Professor Jaramillo also reported a detailed study on the growth of native oxides of 2D MoS_2 and $Zr(S,Se)_2$; this semiconductor technology based on 2D materials will be critically important but remains poorly understood.

In separate work, Professors LeBeau and Jaramillo reported a new paradigm for semiconductor devices based on simulating the response of materials to light but using only electrical stimulation. This new paradigm for electronic devices can be thought of as "photoconductivity without photons" and has been given the technical moniker defect-level switching (DLS), reflecting the atomic-scale operating principle. Unlike established approaches to resistive switching, DLS devices operate without the movement of atoms and can be predictably designed with device simulation software and a thorough understanding of semiconductor defect physics. With further development, DLS devices may find a host of uses in semiconductor technology including circuit protection, resonators, memory devices, and neuromorphic computing.

Professors Gomez-Bombarelli and Olivetti used computational tools for a new study of zeolites (nanoporous inorganic materials) published in *Nature Materials*. Thanks to their low cost, high stability, and finely controlled porous structure, zeolites have broad industrial applications in catalysis and separation. Around 250 metastable zeolitic materials are known, of which 80% are synthetic. In contrast, exhaustive computational enumeration of crystals predicts the existence of hundreds of thousands of nanoporous silica polymorphs. This discrepancy has been referred to as "the zeolite conundrum." Because all zeolites are energetically metastable, their synthesis is governed by kinetics, and complex high-dimensional relationships exist between experimental conditions and a synthesized phase. Many zeolite structures can be converted selectively into others through a number of recrystallization and diffusionless processes. In the latter case, the transformations occur in the solid phase without loss of crystallinity or material. Interzeolite transformations are an exciting avenue to both discover new materials and synthesize known ones more effectively.

The researchers' computational tools identified the key drivers of selectivity in diffusionless interzeolite transformations and postulated new promising transformations. Using automated data extraction and language processing tools, the researchers extracted an exhaustive list of 391 interzeolite transformations from a corpus of 70,000 journal articles. They then used atomic connectivity to represent each material as a 2D graph instead of a traditional 3D crystal. By then comparing the graphs of each pair of materials involved in the transformations, they found that zeolite diffusionless transformations always occur between frameworks with highly similar bond networks, regardless of 3D considerations. Using this criterion, they identified pairs of known frameworks that can potentially be interconverted and numerous transformations that could drive conversions from known to novel so far hypothetical frameworks.

Associate Professor Polina Anikeeva worked with Professor Taşan on a project published in *Science*. Artificial muscles may accelerate the development of robotics, haptics, and prosthetics. Although advances in polymer-based actuators have delivered unprecedented strengths, producing these devices at scale with tunable dimensions

remains a challenge. The researchers applied a high-throughput iterative fiber-drawing technique to create strain-programmable artificial muscles with dimensions spanning three orders of magnitude. These fiber-based actuators are thermally and optically controllable, can lift more than 650 times their own weight, and can withstand strains of over 1,000%. Integration of conductive nanowire meshes within these fiber-based muscles offers piezoresistive strain feedback and demonstrates long-term resilience across more than 10⁵ deformation cycles. The scalable dimensions of these fiber-based actuators and their strength and responsiveness may extend their impact from engineering fields to biomedical applications.

Professor LeBeau received a Presidential Early Career Award for Scientists and Engineers. Professor Julia Ortony received National Science Foundation CAREER funding for her project Fundamentals of Conformational and Surface Water Dynamics in Supramolecular Nanofibers. Among those receiving funding from the MIT Energy Initiative this year were Professor Olivetti and Thomas Lord Associate Professor Jennifer Rupp, who will be participating in a team project (Rapid Material Discovery for Solid-State Batteries: Coupling Low-Cost Processing with Material Screening and Performance Optimization Using Machine Learning), and John F. Elliot Professor of Materials Chemistry Donald R. Sadoway for his project Extremely Low-Cost Aluminum-Sulfur Battery Running Below 100 Degrees Celsius for Grid-Level Energy Storage. Associate Professor Juejun Hu received funding from MIT.nano's NCSOFT seed grants in order to develop high-performance, ultra-thin immersive micro-displays for augmented reality/ virtual reality applications.

Awards and Honors

Associate Professor Alfredo Alexander-Katz and R.P. Simmons Professor of Ceramics and Electronic Materials Harry Tuller have been selected as two of MIT's Committed to Caring professors. Nominations for this honor come from graduate students, who share their experiences as advisees and in the classroom.

Professor Anikeeva was named a Margaret MacVicar Faculty Fellow for her passion for her work, devotion to her students, and creative solutions to educational challenges.

James Mason Crafts Professor Angela Belcher and her research group won first place in the STAT Madness competition for their work concerning new technology to see tiny ovarian cancer tumors in the body.

Kyocera Professor Yet-Ming Chiang was named a fellow of the Electrochemical Society. These fellowships honor advanced individual technological contributions in the fields of electrochemistry and solid state science and technology as well as service to the society.

David H. Koch Professor of Engineering Michael Cima will receive the W. David Kingery Award from the American Ceramic Society. This award, named for a former DMSE faculty member, recognizes lifelong achievements in and multidisciplinary and global contributions to ceramic technology, science, education, and art.

Professor LeBeau was awarded the Burton Medal. This award honors distinguished contributions to the field of microscopy and microanalysis by a scientist who is less than 40 years of age.

In recognition of her distinguished record of contributions to the advancement of archaeological science, the Archaeological Institute of America presented Professor Heather Lechtman with the 2020 Pomerance Award for Scientific Contributions to Archaeology.

Professor Olivetti received the Paul Gray Award from the PKG Center. This award recognizes a member of the MIT faculty who exemplifies building "a better world" through her or his teaching, research, advising, and service.

During the Minerals, Metals & Materials Society (TMS) spring conference in February, Professor Sadoway's 70th birthday was recognized with a symposium titled Process Metallurgy and Electrochemistry of Molten Salts, Liquid Metal Batteries, and Extraterrestrial Materials Processing: An EPD Symposium in Honor of Don Sadoway. To honor Professor Sadoway, collaborators and friends are establishing the TMS Sadoway Materials Innovation and Advocacy Award, which will be presented to a mid-career individual who has made a broad impact in materials science and engineering through education, public advocacy, and entrepreneurship, particularly in areas of sustainability.

Professor Schuh was named a fellow of the National Academy of Inventors in recognition of his meaningful role in bringing about innovations that affect daily life.

Undergraduate Awards

Jeremy Dudo '20 and Danielle Grey-Stewart '20 received the Horace A. Lubin Award for Service to the DMSE Community.

Claire Halloran '20 received the Joseph M. Dhosi Outstanding Internship Award for her work on a project conducted at the University of Oxford (Investigating Li+ Ion Transport in Ionic Liquid Electrolyte EMIFSI to Enable High Specific Energy Li-Metal Batteries).

Lucy Kitch-Peck '22 and Jocelyn Ting '22 were named Outstanding Sophomores.

Isaac Metcalf '20 received the Outstanding Senior Thesis Award for "Searching for Mixed Octahedral-Tetrahedral Interstitial Hydrogen Occupation in Pd-Ti Sublattices: A Computational Study." He also received the Undergraduate Student Teaching Award in Teaching an Undergraduate Subject for 3.091 Introduction to Solid State Chemistry.

Cindy Shi '20 was named Outstanding Senior.

Ava Waitz '21 received the Julian Szekely Award for Outstanding Junior.

Talia Khan '20 was awarded a Fulbright Fellowship that she will use to conduct research in the Brazilian Amazon. She also received MIT's Suzanne Berger Award for Future Global Leaders and a Laya and Jerome B. Wiesner Student Art Award for outstanding achievement in and contributions to the arts at MIT.

Wesley Block '22 received the Harold J. Pettegrove Award, which honors outstanding service to intramural athletics.

Neosha Narayanan '21 and Avery Nguyen '21 were selected as Burchard Scholars for their demonstrated academic excellence in both humanities and science, technology, engineering, and mathematics (STEM) fields.

Caleb Richardson '20 was the recipient of the Ronald E. McNair Scholarship Award, which recognizes a Black undergraduate who has demonstrated strong academic performance and made contributions to the minority community.

Claire Halloran, Yiran He '20, Isaac Metcalf, Cindy Shi, and Hilary Vogelbaum '20 were all invited to join Phi Beta Kappa.

Claire Halloran was named a 2020 Rhodes Scholar. At Oxford, she will pursue an MSc in energy systems and a master of public policy.

Isaac Metcalf was awarded a Hertz Fellowship from the Fannie and John Hertz Foundation. He will pursue graduate studies at Rice University in the fall.

Pooja Reddy '20 received a Paul and Daisy Soros Fellowship for New Americans. In the fall, Pooja will begin work on a PhD in materials science and engineering at Stanford University.

Graduate Awards

Akash Bajaj received the John Wulff Award for Excellence in Teaching for his work as a teaching assistant in 3.012 Fundamentals of Materials Science.

Eunsoo Cho won the Exceptional First-Year Performance Award.

Ty Christoff-Tempesta was presented the Graduate Student Community Service Award.

Margaret Lee received the Graduate Student Teaching Award in Teaching a Graduate Subject for her work as a teaching assistant in 3.65 Soft Matter Characterization.

P.J. Santos won the Best PhD Thesis Award for "Self-Assembling Nanocomposite Tectons for Ordered Superlattices."

Daniel Schwalbe-Koda was presented the Best Paper Award by a First- or Second-Year Student for "Graph Similarity Drives Zeolite Diffusionless Transformations and Intergrowth," which was published in *Nature Materials*.

Kate Reidy was awarded a Mathworks Fellowship for her use of MATLAB in her materials research.

Staff Awards

Senior financial administrator Kariuki Thande received an Infinite Mile Award from the School of Engineering this spring in recognition of his outstanding work and leadership.

Greg Ekchian, a postdoc in Professor Cima's group, was recognized with a TR35 Award. Also, he received a Blavatnik Fellowship in Life Science Entrepreneurship to spend the 2021 academic year at Harvard Business School.

Future Plans

Work on revising the graduate curriculum continues, with Frances Ross now leading the departmental committee on graduate students. We expect a new faculty hire in computational materials science to begin in January 2021.

In response to national events and community demand, DMSE will soon create a DEI council and will create the position of a DEI officer who will work with faculty, students, and staff on many issues.

Jeffrey C. Grossman Department Head Morton and Claire Goulder and Family Professor in Environmental Systems Professor of Materials Science and Engineering