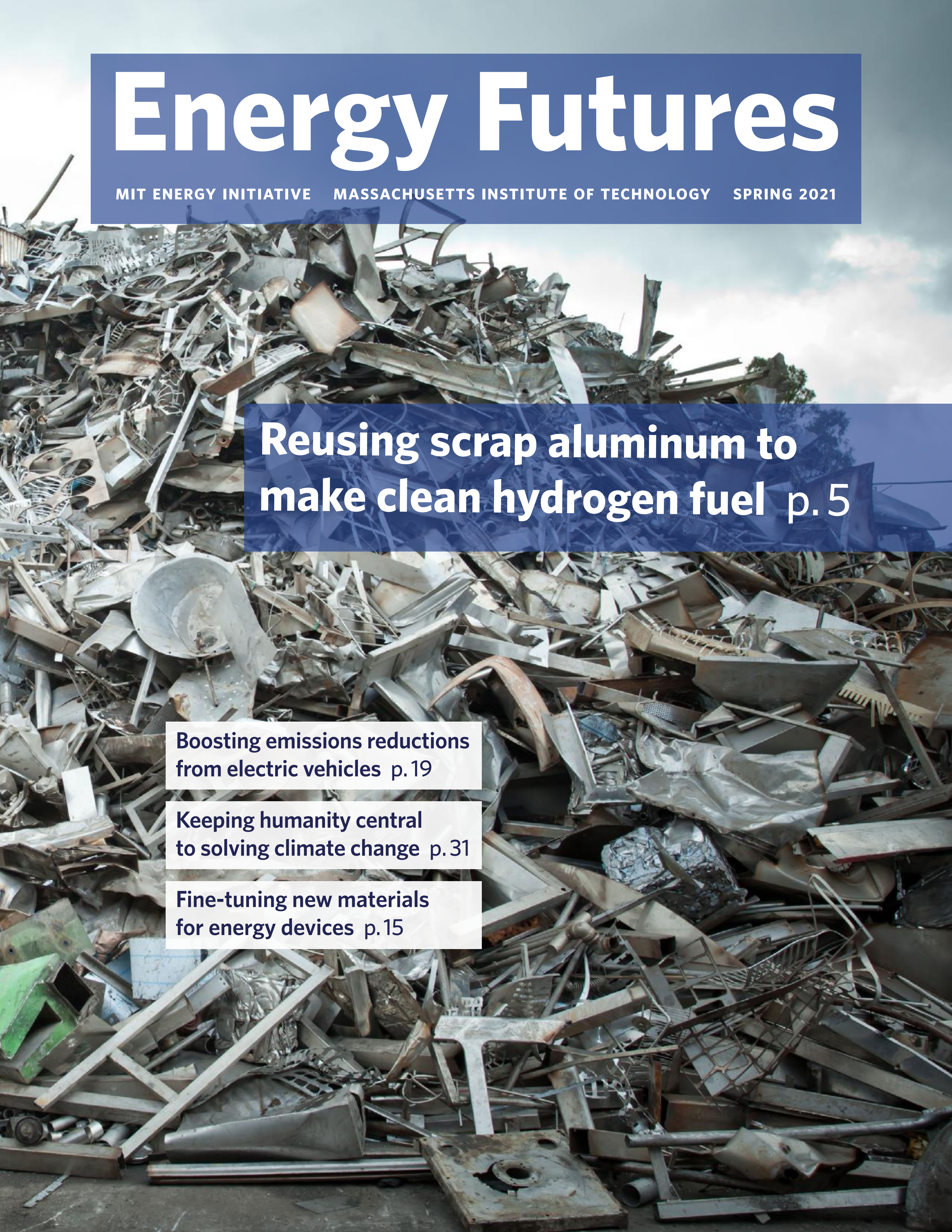

Energy Futures

MIT ENERGY INITIATIVE MASSACHUSETTS INSTITUTE OF TECHNOLOGY SPRING 2021

MIT Energy Initiative podcast

Recent episodes of the MITEI podcast include the following:

Building technology
Jessica Granderson, staff scientist and deputy of research programs for the Building Technology and Urban Systems Division at Lawrence Berkeley National Laboratory, talks about building analytics, energy efficiency, and the grid.

Cost of car ownership
David Keith, assistant professor at the MIT Sloan School, and Joanna Moody, research program manager at MITEI's Mobility Systems Center, discuss why we value our cars and what it means for sustainable urban mobility in the future.

The science of solar
Frank van Mierlo, CEO of 1366 Technologies, talks about the science of solar, green hydrogen, and an unexpected skill resulting from an MIT education.

Energy and filmmaking
Scott Tinker, director of the Bureau of Economic Geology, professor at the University of Texas at Austin, and founder and chairman of Switch Energy Alliance, describes energy and filmmaking in the developing world.

Digitalization and the power grid
Mark Thompson, director of digital delivery at National Grid, discusses digitalization, industry standards, and the day-to-day of how the grid is being converted to renewable energy.

America's largest municipal utility
Paula Gold-Williams, president and CEO of CPS Energy, which serves San Antonio, Texas, and surrounding communities, talks about running the nation's largest municipally owned gas and electric utility.

Energy access in Africa and beyond
Damilola Ogunbiyi, CEO of Sustainable Energy for All and co-chair of UN-Energy, discusses energy access, electrification in Nigeria, and the power of data.

…and more

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Awards

MITEI Director Robert C. Armstrong receives prestigious AIChE award

In autumn 2020, MITEI Director Robert C. Armstrong, the Chevron Professor of Chemical Engineering, received the 2020 American Institute of Chemical Engineers' Founders Award for Outstanding Contributions to the Field of Chemical Engineering in honor of his landmark contributions to chemical engineering research and education, and for leadership in advancing the transition to a low-carbon future and addressing climate change. AIChE is the world's leading organization for chemical engineering professionals, with more than 60,000 members from more than 110 countries. For more information, go to www.aiche.org/community/bio/robert-c-armstrong.

On the cover
MIT researchers have shown that pieces of aluminum often found in scrap piles such as this one can be easily transported and used to generate clean hydrogen fuel at any location with available water. They developed guidelines on how to select and prepare scraps of specific aluminum alloys to produce a hydrogen flow that will match the demand of a particular device or system. See page 5.
Photo: StockStudio/Alamy Stock Photo

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Nancy W. Stauffer, editor
stauffer@mit.edu

Kelley Travers, assistant editor
ktravers@mit.edu

Tom Melville, MITEI communications director
thomasme@mit.edu

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MIT Energy Initiative
Massachusetts Institute of Technology
77 Massachusetts Avenue, E19-307
Cambridge, MA 02139-4307

617-258-8891

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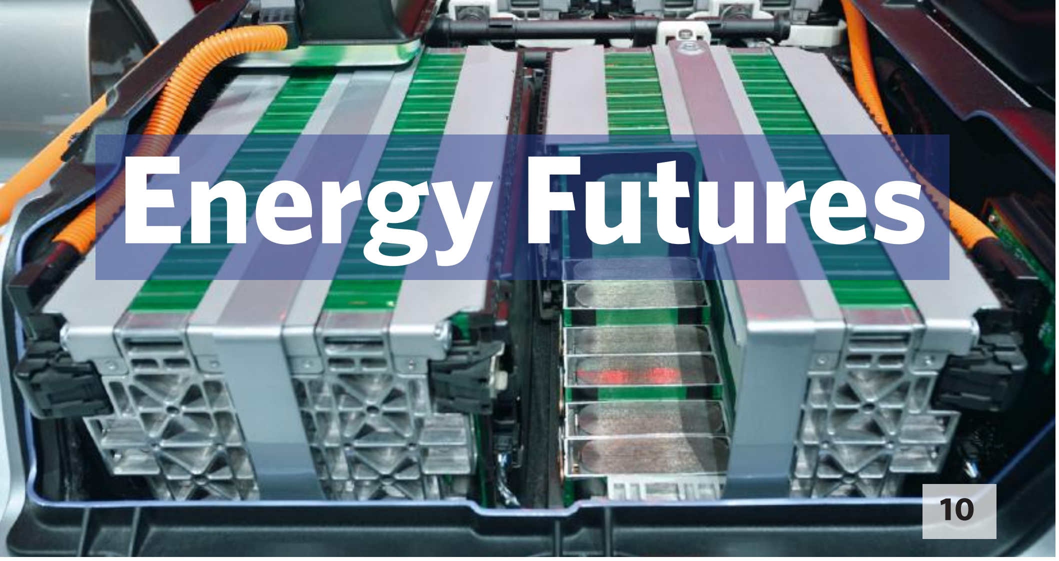


Spring 2021

MITei
MIT Energy Initiative

Massachusetts Institute
of Technology

A letter from the director

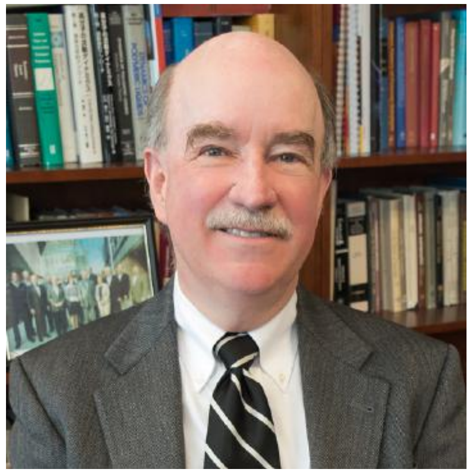
Dear friends,

It has now been more than a year since MIT and the rest of the world locked down in an effort to slow the spread of Covid-19. In that time, we have experienced grief and tragedy, but also extreme determination and perseverance. At MITEI, we have been humbled by the creativity and dedication of our community, which, despite many obstacles, remains committed to educating our students and finding clean energy solutions.

MIT has worked hard to keep programs running and to bring our researchers back to their labs as quickly and—most importantly—as safely as possible. MITEI looks forward to joining our colleagues on campus in what will be the "new normal" in the coming academic year.

The Institute continues to prioritize climate action, empowering our researchers to think collaboratively and strategically about where we need to make more ambitious efforts to move the needle on climate change. In March, MITEI co-hosted an engagement forum that gave the MIT community an opportunity to learn about and offer thoughts on the benefits and challenges of working with organizations outside of the Institute (page 44). As MIT Vice President for Research Maria T. Zuber said in her remarks, "MIT can't solve climate change alone." This event, which highlighted the benefits of these research collaborations, was part of a multiyear process informing the next phase of MIT's climate action plan, which is being announced this spring.

From designs for a hybrid-electric plane (page 21) to steps you can take to reduce the environmental footprint of your internet usage (page 23) to new models rethinking the hydrogen supply chain (page 29), MIT researchers truly embody



MITEI's research, education, and outreach programs are spearheaded by Professor Robert C. Armstrong, director. Photo: Kelley Travers, MITEI

the Institute's motto "mens et manus," or "mind and hand." This issue of *Energy Futures* highlights several of these innovative technologies and solutions that can help decarbonize our energy systems and accelerate climate change mitigation.

On page 5, you will read about a technique to generate hydrogen by reacting scrap aluminum and water, demonstrating that aluminum can be a high-energy-density, easily transportable, flexible, and carbon-free source of hydrogen. In this issue, you will also read about researchers who have developed an approach for designing solid-state batteries that could be key to widespread adoption of electric vehicles and a major step in decarbonizing the transportation sector (page 10), as well as about important insights into a remarkable class of materials called metal-organic frameworks that could advance a variety of energy-related technologies (page 15).

This issue will also introduce you to gifted scholars in MIT's School of Humanities, Arts, and Social Sciences, whose research and ideas can help solve the economic, cultural, and political dimensions of the world's energy and climate challenges (page 31). At the heart of any technological solution are the people who will need to implement, advocate, support, use, and, eventually, even dispose of it. This past fall, Professor Clapperton Chakanetsa Mavhunga taught a course that focused on the environmental and health consequences of improperly discarded electronics waste—a huge issue as more and more of our innovations age into obsolescence (page 34).

With a heavy heart, I share with you the passing of three members of our MITEI community. We mourn the loss of George P. Shultz PhD '49, who chaired our External Advisory Board from its beginning until he stepped down as chair at age 98 (but graciously remained on the board). He was a fierce advocate for climate change action and provided invaluable guidance on our work. You can read more about his life and contributions on page 3. I am also sorry to share the passing of Stephen D. Bechtel, Jr., and John M. Bradley '47, SM '49. Stephen was an inaugural member of our External Advisory Board and a champion of our undergraduate students and courses. John supported our Seed Fund Program and loved engaging in the science and technical details of the novel energy research projects it generates. They will be missed dearly.

I want to thank you for reading this issue of *Energy Futures* and for your support. Please stay safe and healthy, and keep in touch.

Warm regards,

Robert C Armstrong

Professor Robert C. Armstrong
MITEI Director
April 2021

George P. Shultz PhD '49 (1920–2020)

George P. Shultz PhD '49, former U.S. secretary of labor, state, and of the treasury, died peacefully at his home in Stanford, California, on February 6, 2020, at the age of 100. A champion of bipartisanship who for decades urged action on climate change, he leaves a rich legacy forged during more than 70 years of leadership in government, academia, and business.

George P. Shultz PhD '49 (left) and MITEI Director Robert C. Armstrong at a March 2013 meeting in Washington, D.C., where MIT and Stanford University's Hoover Institution held a workshop on game-changing technologies to achieve sustained economic growth and address energy and climate challenges. Photo: Jay Mallin

"A beloved teacher, a brilliant scholar, a visionary leader, a public servant of the highest integrity, and a relentless champion for the breakthrough energy technologies on which the future of our society depends, George Shultz represented the very best of MIT and of our nation," says MIT President L. Rafael Reif. "We will remember Secretary Shultz for the boundless energy, piercing clarity, and innovative ideas he brought to every role and every conversation. And we are profoundly grateful for the eloquence of his example: a life lived in service to the common good."

Born in New York City on December 13, 1920, Shultz grew up in Englewood, New Jersey. He graduated from Princeton University in 1942. He was admitted to MIT for a master's degree program and planned to enroll in 1943, but he paused his academic pursuits to enlist in the U.S. Marine Corps during World War II. He served from 1942 to 1945, rising to the rank of captain.

Following his military service, Shultz began what would become more than a decade of scholarship and teaching at MIT. After earning his PhD in industrial economics, he taught economics at the Institute in the Department of Economics and at the Sloan School of Management, first as an assistant professor, then as an associate professor.

"George and I were assistant professors together. That was seventy years ago," says Robert M. Solow, a professor emeritus of economics. "We remained friends ever after. Even once he got used to being in high office, there was always a bit of that young researcher in him. I can remember his going door to door in Nashua, New Hampshire, learning about the lives of the unemployed. Everyone will miss him."

In 1955, he took a leave of absence from MIT to serve as a senior staff economist on President Dwight D. Eisenhower's Council of Economic Advisers. From 1957 to 1968, he served at University of Chicago Graduate School of Business as a professor of industrial relations and then as the school's dean.

He was appointed U.S. secretary of labor under President Richard Nixon in 1969; in this role, he prioritized poverty reduction and equal employment opportunities, among other initiatives. In 1970, he became the first director of the Office of Management and Budget, a Cabinet-level office, where he worked to advance school desegregation efforts. He then served as U.S. secretary of the treasury, where he co-founded the international organization that later became known as the Group of Seven (G7) nations, formed to pursue shared economic objectives. Shultz served as chairman of the President's Economic Policy Advisory Board from 1981 to 1982. In the private sector, he held executive roles at Bechtel Group, Inc., from 1974 to 1982.

He is perhaps best known for his tenure as U.S. secretary of state under President Ronald Reagan, from 1982 to 1989. Shultz was a key figure in facilitating the de-escalation of tensions between the U.S. and the Soviet Union, helping to draft agreements that led to the end of the Cold War. In 1989, he received the Presidential Medal of Freedom, the nation's highest civilian honor. From 1989 until his death, he was a distinguished fellow at Stanford University's Hoover Institution.

Shultz's affiliation with MIT remained strong over the years. When accepting the Robert A. Muh Award for noteworthy achievement in the humanities, arts, and social sciences at MIT in 2003, Shultz gave a talk on national security. He asserted that "as a country, we need to do things that are broadly beneficial to the world."

This philosophy extended to topics including climate change and the transition to low-carbon energy. In recent decades, Shultz became an outspoken advocate for farsighted action to address climate change. He urged the U.S. to cut its dependence on oil in favor of clean energy production, championed sustained federal support for basic research, and built bipartisan support for a revenue-neutral carbon tax proposal—ideas he advocated publicly and discussed over the years with the MIT community.

In 2007, as the Institute was launching the MIT Energy Initiative (MITEI), he became the inaugural chair of its External Advisory Board, a leadership role he held until 2019, when he chose to step down as chair. He remained a member of the board until his death, working closely with his successor and longtime friend Norman Augustine.

"George inspired those of us working on clean energy and climate change. It was a pleasant surprise when he agreed to be the inaugural chair of the MIT Energy Initiative's External Advisory Board and, because of his enthusiasm, we didn't need a second chair for a dozen years!" says Ernest J. Moniz, professor emeritus of physics post-tenure, thirteenth U.S. secretary of energy, and the founding director of MITEI. "I am deeply saddened by the loss of this remarkable statesman and friend."

"Secretary Shultz was generous with his time, his wisdom, and his friendships, creating critically needed communities of shared concern—which he recognized was the way to get things done, and to have lots of fun doing so," says MIT President Emerita Susan Hockfield. "As founding chair of the External Advisory Board of MIT's Energy Initiative, Secretary Shultz integrated the insights of industry with the ambitions of the academy, to apply lab-based discoveries to the pressing problem of climate change. He made MITEI and MIT better, and we all enjoyed every minute of the time he shared with us."

Former U.S. Secretary of State George P. Shultz PhD '49 (left) and MIT President L. Rafael Reif at the 2019 meeting of the MIT Energy Initiative External Advisory Board. Photo: Eric Haynes

"George taught us much about the importance of a principled vision coupled with persistence in engaging with government on the energy and climate challenge," says MITEI Director Robert C. Armstrong. "He also reminded us to focus on the hard problems like energy in the developing world—which led to our launch of the Tata Center for Technology and Design and other initiatives since then. We will miss him and his guidance greatly here at MITEI."

"George Shultz is the iconic example of the contributions MIT individuals make to the country. We should honor his memory by producing many more," says John Deutch, Institute Professor Emeritus and former U.S. director of Central Intelligence who held numerous leadership positions in the U.S. Department of Defense and U.S. Department of Energy.

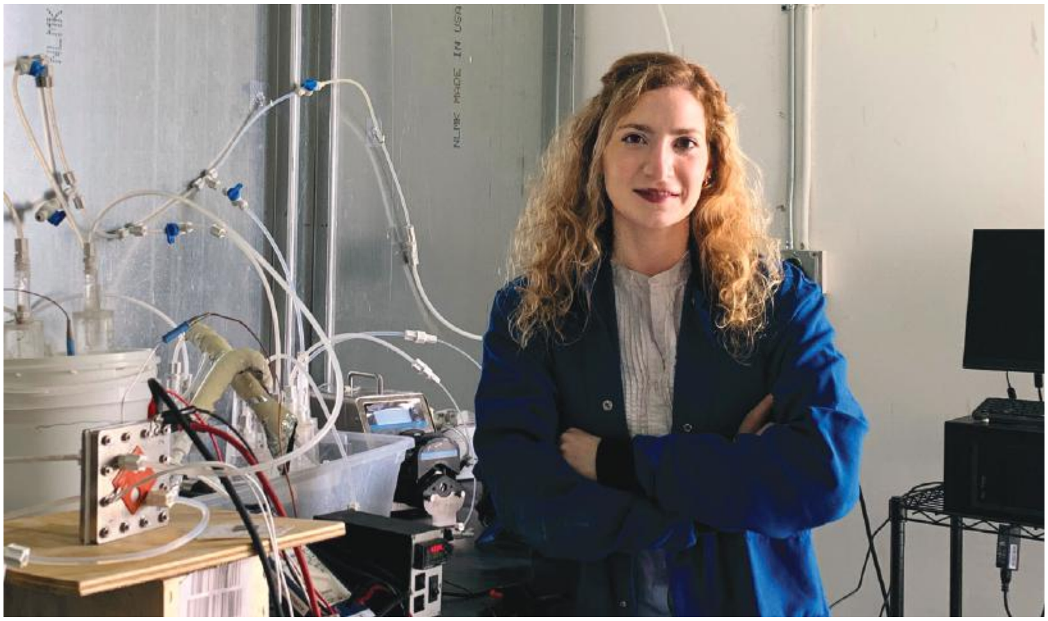
Christopher Knittel, the George P. Shultz Professor of Applied Economics at the Sloan School, says, "It is a tremendous honor to hold the George P. Shultz chair, and I feel privileged to have known George, whose wit, wisdom, and statesmanship were unmatched and irreplaceable. I will miss our conversations spanning climate policy to mainstream economics research. Rest in peace, Secretary Shultz."

Shultz authored numerous articles and books, including *Turmoil and Triumph: My Years as Secretary of State* (1993), *Learning from Experience* (2016), and *Thinking about the Future* (2019). He was an editor of *Beyond Disruption: Technology's Challenge to Governance* (2018). His most recent book, *Hinge of History: Governance in an Emerging New World*, was published in November 2020.

Shultz's remarkable life was built on the foundation of two long marriages. He and his first wife, Lieutenant Helena "O'Bie" O'Brien, a military nurse, met while stationed in Hawaii during the war. The couple raised five children together and were married until her death in 1995. He later married Charlotte Mailliard Swig, the City of San Francisco's chief of protocol; they were married for 23 years until his death. In addition to Swig, his survivors include his children, 11 grandchildren, and nine great-grandchildren.

He will be deeply missed by his family, colleagues, students, and friends around the world, many of whom shared warm wishes virtually for his 100th birthday celebration in December 2020. To mark the occasion, Shultz wrote in *The Washington Post* about 10 things he'd learned about trust in his 100 years, underscoring the importance of developing, maintaining, and rebuilding our trust in each other. "Trust is fundamental, reciprocal and, ideally, pervasive. If it is present, anything is possible. If it is absent, nothing is possible," he wrote.

Emily Dahl, MITEI



Using aluminum and water to make clean hydrogen fuel—when and where it's needed

Nancy W. Stauffer, MITEI

IN BRIEF

MIT researchers have produced practical guidelines for generating hydrogen using scrap aluminum and water. First, they obtained specially fabricated samples of pure aluminum and aluminum alloys designed to replicate the types of scrap aluminum typically available from recycling sources. They then demonstrated ways of treating the samples to ensure that the surfaces of all the aluminum "grains" that make up the solid remain free of deposits throughout the reaction. Next, they showed that they could "tune" the hydrogen output by starting with pure aluminum or specific alloys and by manipulating the size of the internal aluminum grains. Such tuning can be used to meet demands for brief bursts of hydrogen, for example, or for lower, longer-lasting flows. The work confirms that, when combined with water, aluminum can provide a high-energy-density, easily transportable, flexible source of hydrogen to serve as a carbon-free replacement for fossil fuels.

As the world works to move away from fossil fuels, many researchers are investigating whether clean hydrogen fuel can play an expanded role in sectors from transportation and industry to buildings and power generation. It could be used in fuel cell vehicles, heat-producing boilers, electricity-generating gas turbines, systems for storing renewable energy, and more.

But while using hydrogen doesn't generate carbon emissions, making it typically does. Today, almost all hydrogen is produced using fossil fuel–based processes that together generate more than 2% of

Above Laureen Meroueh PhD '20 (pictured) and Professors Douglas P. Hart and Thomas W. Eagar have systematically studied how to generate hydrogen by combining aluminum with water. Their results show that by choosing a specific aluminum alloy from a waste heap and taking a few steps to modify it, a user can generate the flow of hydrogen needed for a particular practical application. Photo: Reza Mirshekari all global greenhouse gas emissions. In addition, hydrogen is often produced in one location and consumed in another, which means its use also presents logistical challenges.

A promising reaction

Another option for producing hydrogen comes from a perhaps surprising source: reacting aluminum with water. Aluminum metal will readily react with water at room temperature to form aluminum hydroxide and hydrogen. That reaction doesn't typically take place because a layer of aluminum oxide naturally coats the raw metal, preventing it from coming directly into contact with water.

Using the aluminum-water reaction to generate hydrogen doesn't produce any greenhouse gas emissions, and it promises to solve the transportation problem for any location with available water. Simply move the aluminum and then react it with water on-site. "Fundamentally, the aluminum becomes a mechanism for storing hydrogen—and a very effective one," says Douglas P. Hart, professor of mechanical engineering. "Using aluminum as our source, we can 'store' hydrogen at a density that's 10 times greater than if we just store it as a compressed gas."

Two problems have kept aluminum from being employed as a safe, economical source for hydrogen generation. The first problem is ensuring that the aluminum surface is clean and available to react with water. To that end, a practical system must include a means of first modifying the oxide layer and then keeping it from re-forming as the reaction proceeds.

The second problem is that pure aluminum is energy-intensive to mine and produce, so any practical approach needs to use scrap aluminum from various sources. But scrap aluminum is not an easy starting material. It typically occurs in an alloyed form, meaning that it contains other elements that are added to change the properties or characteristics of the aluminum for different uses. For example, adding magnesium increases strength and corrosion-resistance, adding silicon lowers the melting point, and adding a little of both makes an alloy that's moderately strong and corrosion-resistant.

Despite considerable research on aluminum as a source of hydrogen, two key questions remain: What's the best way to prevent the adherence of an oxide layer on the aluminum surface, and how do alloying elements in a piece of scrap aluminum affect the total amount of hydrogen generated and the rate at which it is generated?

"If we're going to use scrap aluminum for hydrogen generation in a practical application, we need to be able to better predict what hydrogen generation characteristics we're going to observe from the aluminum-water reaction," says Laureen Meroueh PhD '20 of mechanical engineering.

Since the fundamental steps in the reaction aren't well understood, it's been hard to predict the rate and volume at which hydrogen forms from scrap aluminum, which can contain varying types and concentrations of alloying elements. So Hart, Meroueh, and Thomas W. Eagar SB '72, ScD '75, a professor of materials engineering and engineering management in the Department of Materials Science and Engineering, decided to examine—in a systematic fashion—the impacts of those alloying elements on the aluminum-water reaction and on a promising technique for preventing the formation of the interfering oxide layer.

To prepare, they had experts at Novelis Inc. (Spokane, Washington) fabricate samples of pure aluminum and of specific aluminum alloys made of commercially pure aluminum combined with either 0.6% silicon (by weight), 1.0% magnesium, or both—compositions that are typical of scrap aluminum from a variety of sources. Using those samples, the MIT researchers performed a series of tests to explore different aspects of the aluminum-water reaction.

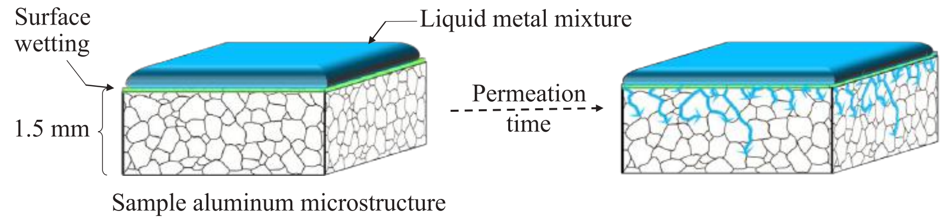
Pretreating the aluminum

The first step was to demonstrate an effective means of penetrating the oxide layer that forms on aluminum in the air. Solid aluminum is made up of tiny grains that are packed together with occasional boundaries where they don't line up perfectly. To maximize hydrogen production, researchers would need to prevent the formation of the oxide layer on all those interior grain surfaces.

Research groups have already tried various ways of keeping the aluminum grains "activated" for reaction with water. Some have crushed scrap samples into particles so tiny that the oxide layer doesn't adhere. But aluminum powders are dangerous, as they can react with humidity and explode. Another approach calls for grinding up scrap samples and adding liquid metals to prevent oxide deposition. But grinding is a costly and energy-intensive process.

To Hart, Meroueh, and Eagar, the most promising approach—first introduced by Jonathan Slocum ScD '18 while he was working in Hart's research group—involved pretreating the solid aluminum by painting liquid metals on top and allowing them to permeate through the grain boundaries, as shown in the diagram on page 7.

To determine the effectiveness of that approach, the researchers needed to confirm that the liquid metals would reach the internal grain surfaces, with and without alloying elements present. And they had to establish how long it would take for the liquid metal to coat all of the grains in pure aluminum and its alloys.



Preventing the formation of an oxide coating
To enable the hydrogen-forming reaction to occur, the researchers must first disrupt the naturally occurring oxide coating that's on the surface of the aluminum and then make sure it doesn't re-form as the aluminum and water react. To that end, they paint the surface of the solid with a carefully designed room-temperature liquid metal mixture. The mixture initially wets the surface; but over time, it permeates through the grain boundaries and reaches the interior grain surfaces, as illustrated above.

They started by combining two metals—gallium and indium—in specific proportions to create a "eutectic" mixture, that is, a mixture that would remain in liquid form at room temperature. They coated their samples with the eutectic and allowed it to penetrate for time periods ranging from 48 to 96 hours. They then exposed the samples to water and monitored the hydrogen yield (the amount formed) and flow rate for 250 minutes. After 48 hours, they also took high-magnification scanning electron microscope (SEM) images so they could observe the boundaries between adjacent aluminum grains.

Based on the hydrogen yield measurements and the SEM images, the MIT team concluded that the gallium-indium eutectic does naturally permeate and reach the interior grain surfaces. However, the rate and extent of penetration vary with the alloy. The permeation rate was the same in silicon-doped aluminum samples as in pure aluminum samples but slower in magnesium-doped samples.

Perhaps most interesting were the results from samples doped with both silicon and magnesium—an aluminum alloy often found in recycling streams. Silicon and magnesium chemically bond to form magnesium silicide, which occurs as solid deposits on the internal grain surfaces. Meroueh hypothesized that when both silicon and magnesium are present in scrap aluminum, those deposits can act as barriers that impede the flow of the gallium-indium eutectic.

The experiments and images confirmed her hypothesis: The solid deposits did act as barriers, and images of samples pretreated for 48 hours showed that permeation wasn't complete. Clearly, a lengthy pretreatment period would be critical for maximizing the hydrogen yield from scraps of aluminum containing both silicon and magnesium.

Meroueh cites several benefits to the process they used. "You don't have to apply any energy for the gallium-indium eutectic to work its magic on aluminum and get rid of that oxide layer," she says. "Once you've activated your aluminum, you can drop it in water, and it'll generate hydrogen—no energy input required." Even better, the eutectic doesn't chemically react with the aluminum. "It just physically moves around in between the grains," she says. "At the end of the process, I could recover all of the gallium and indium I put in and use it again"—a valuable feature as gallium and (especially) indium are costly and in relatively short supply.

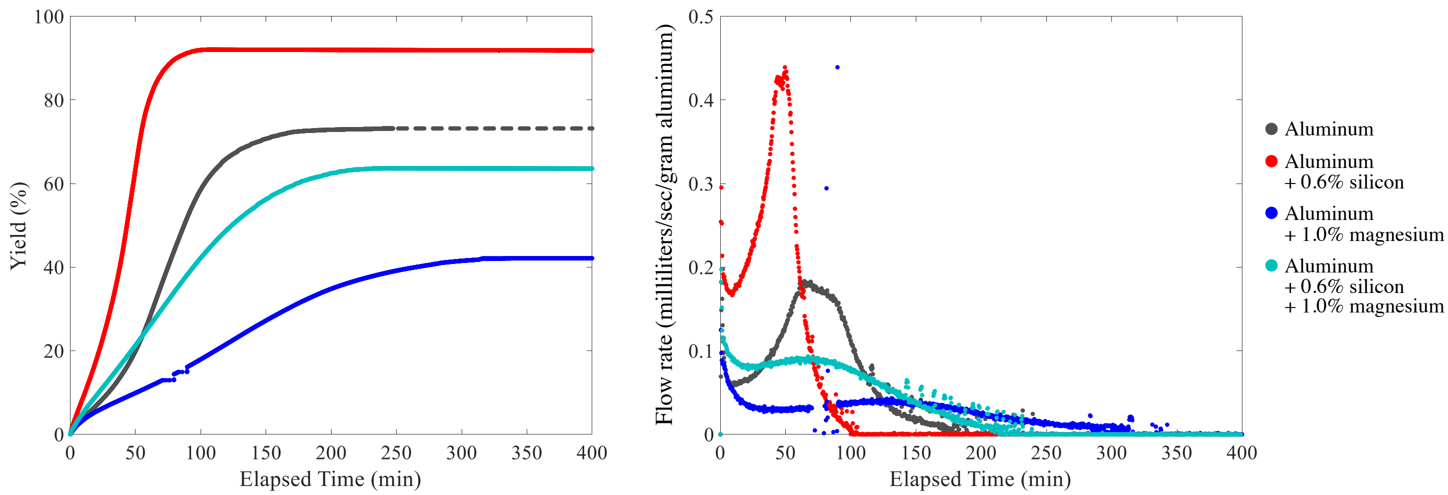
Impacts of alloying elements on hydrogen generation

The researchers next investigated how the presence of alloying elements affects hydrogen generation. They tested samples that had been treated with the eutectic for 96 hours; by then, the hydrogen yield and flow rates had leveled off in all the samples. The figures on page 8 show the impacts on total hydrogen yield (left) and flow rate (right) over time.

As seen in the left-hand figure, the presence of 0.6% silicon (the red curve) increased the hydrogen yield for a given weight of aluminum by 20% compared to pure aluminum (black)—even though the silicon-containing sample had less aluminum than the pure aluminum sample. In contrast, the presence of 1.0% magnesium (dark blue) produced far less hydrogen, while adding both silicon and magnesium (light blue) pushed the yield up but not to the level of pure aluminum.

The right-hand figure shows that the presence of silicon also greatly accelerated the reaction rate, producing a far higher peak in the flow rate but cutting short the duration of hydrogen output. The presence of magnesium produced a lower flow rate but allowed the hydrogen output to remain fairly steady over time. And once again, aluminum with both alloying elements produced a flow rate between that of magnesium-doped and pure aluminum.

Those results provide practical guidance on how to adjust the hydrogen output to match the operating needs of a hydrogen-consuming device. If the starting material is commercially pure aluminum, adding small amounts of carefully selected alloying elements can tailor the hydrogen yield and flow rate. If the starting material is scrap aluminum, careful choice of the source can be key. For high, brief bursts of hydrogen, pieces of silicon-containing aluminum from an auto junkyard could work well. For lower but longer flows, magnesium-containing scraps from the frame of a demolished building might be better. For results somewhere in between, aluminum containing both silicon and magnesium should work well; such material is abundantly available from scrapped cars



Impacts of alloying elements on hydrogen generation
The figures above show the impacts of alloying elements commonly found in scrap aluminum on hydrogen yield (left) and on the rate at which hydrogen is produced (right). The results demonstrate that the hydrogen output can be tuned to match the needs of a particular application. Note that all samples were pretreated with the eutectic for 96 hours before the experiments.

and motorcycles, yachts, bicycle frames, and even smartphone cases.

It should also be possible to combine scraps of different aluminum alloys to tune the outcome, notes Meroueh. "If I have a sample of activated aluminum that contains just silicon and another sample that contains just magnesium, I can put them both into a container of water and let them react," she says. "So I get the fast ramp-up in hydrogen production from the silicon and then the magnesium takes over and has that steady output."

Another opportunity for tuning: Reducing grain size

Another practical way to affect hydrogen production could be to reduce the size of the aluminum grains—a change that should increase the total surface area available for reactions to occur.

To investigate that approach, the researchers requested specially customized samples from their supplier. Using standard industrial procedures, the Novelis experts first fed each sample through two rollers, squeezing it from the top and bottom so that the internal grains were flattened. They then heated each sample until the long, flat grains had reorganized and shrunk to a targeted size.

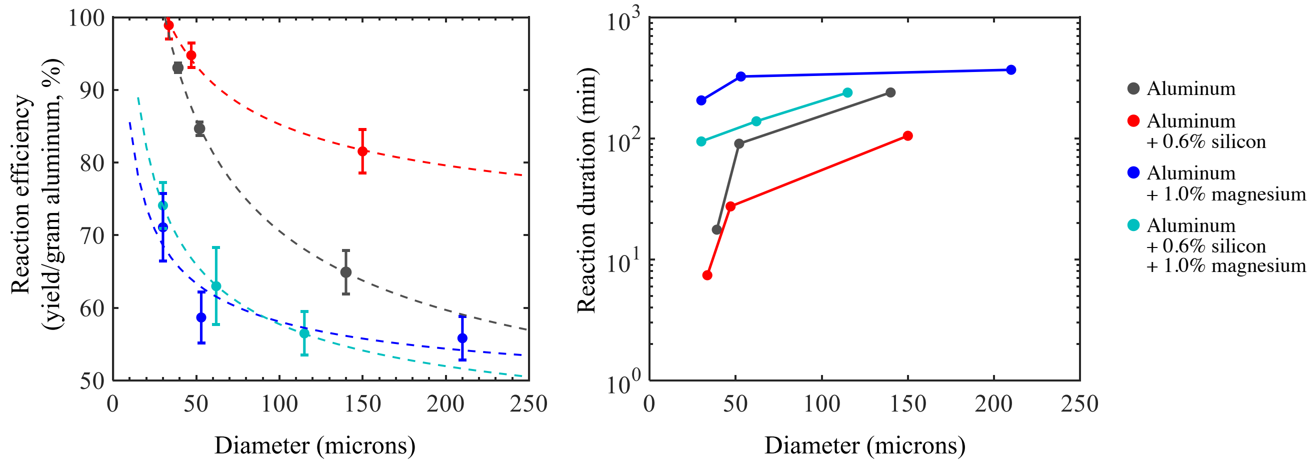
The figures on page 9 present results of decreasing grain size. The left-hand figure shows the change in reaction efficiency, defined as the amount of hydrogen formed per gram of aluminum as a percentage of the theoretical maximum. The curves display results calculated using a widely accepted equation that relates yield strength to grain size. The right-hand figure shows the change in reaction duration. As the figures demonstrate, reducing the grain size increased the efficiency and decreased the duration of the reaction to varying degrees in the different samples.

Needed: A revised theory that explains observations

Throughout their experiments, the researchers encountered some unexpected results. For example, standard corrosion theory predicts that pure aluminum will generate more hydrogen than silicon-doped aluminum will—the opposite of what they observed in their experiments.

To shed light on the underlying chemical reactions, Hart, Meroueh, and Eagar investigated hydrogen "flux," that is, the volume of hydrogen generated over time on each square centimeter of aluminum surface, including the interior grains. They examined three grain sizes for each of their four compositions and collected thousands of data points measuring hydrogen flux.

Their results show that reducing grain size has significant effects. It increases the peak hydrogen flux from silicon-doped aluminum as much as 100 times and from the other three compositions by 10 times. With both pure aluminum and silicon-containing aluminum, reducing grain size also decreases the delay before the peak flux and increases the rate of decline afterward. With magnesium-containing aluminum, reducing the grain size brings about an increase in peak hydrogen flux and results in a slightly faster decline in the rate of hydrogen output. With both silicon and magnesium present, the hydrogen flux over time resembles that of magnesium-containing aluminum when the grain size is not manipulated. When the grain size is reduced, the hydrogen output characteristics begin to resemble behavior observed in silicon-containing aluminum. That outcome was unexpected because when silicon and magnesium are both present, they react to form magnesium silicide, resulting in a new type of aluminum alloy with its own properties.



Impacts of reduction in grain size on two measures
The left-hand figure above shows the change in reaction efficiency, calculated as the yield per gram of aluminum as a percentage of the theoretical maximum. The right-hand figure shows the duration of the reaction in minutes. Again, the presence of particular alloying elements has a major effect on the impact of reducing grain size.

The researchers stress the benefits of developing a better fundamental understanding of the underlying chemical reactions involved. In addition to guiding the design of practical systems, it might help them find a replacement for the expensive indium in their pretreatment mixture. Other work has shown that gallium will naturally permeate through the grain boundaries of aluminum. "At this point, we know that the indium in our eutectic is important, but we don't really understand what it does, so we don't know how to replace it," says Hart.

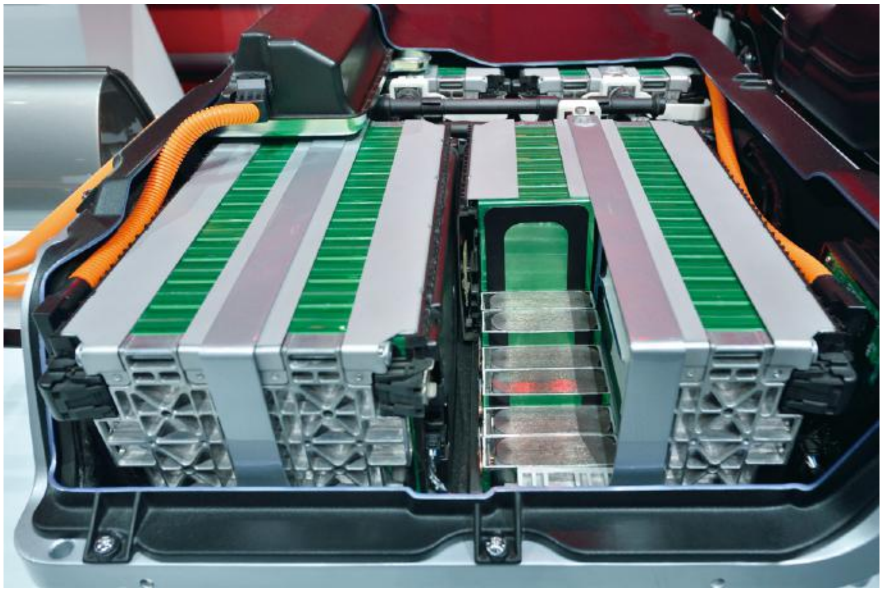
But already Hart, Meroueh, and Eagar have demonstrated two practical ways of tuning the hydrogen reaction rate: by adding certain elements to the aluminum and by manipulating the size of the interior aluminum grains. In combination, those approaches can deliver significant results. "If you go from magnesium-containing aluminum with the largest grain size to silicon-containing aluminum with the smallest grain size, you get a hydrogen reaction rate that differs by two orders of magnitude," says Meroueh. "That's huge if you're trying to design a real system that would use this reaction."

NOTES

This research was supported through the MIT Energy Initiative by ExxonMobil-MIT Energy Fellowships awarded to Laureen Meroueh PhD '20 from 2018 through 2020. Meroueh is now CEO of Alchemr, Inc., a startup that is developing the next generation of scalable water electrolyzers for low-cost green hydrogen production. Further information about the research can be found in:

L. Meroueh, T.W. Eagar, and D.P. Hart. "Effects of Mg and Si doping on hydrogen generation via reduction of aluminum alloys in water." *ACS Applied Energy Materials*, vol. 3, no. 2, pp. 1860–1868, 2020. Online: doi.org/10.1021/acsaem.9b02300.

L. Meroueh, L. Neil, T.W. Eagar, and D.P. Hart. "Leveraging grain size effects on hydrogen generated via doped aluminum-water reactions enabled by a liquid metal." *ACS Applied Energy Materials*, December 2020. Online: doi.org/10.1021/acsaem.0c02175.



Designing better batteries for electric vehicles

Materials selection for scaled-up production

Nancy W. Stauffer, MITEI

IN BRIEF

Worldwide, researchers are working to adapt the standard lithium-ion battery to make versions that are better suited for use in electric vehicles because they are safer, smaller, and lighter—and still able to store abundant energy. An MIT-led study shows that as researchers consider what materials may work best in their solid-state batteries, they also may want to consider how those materials could impact large-scale manufacturing. In some cases, scaled-up production can lead to problems with resource availability or supply chains, high costs due to processing requirements or difficult battery fabrication steps, or costly measures needed to ensure high performance in the final product. Using the approach described in the MIT study, researchers can choose materials that bring the desired result in their benchtop test models while also proving suitable for large-scale production in the future.

The urgent need to cut carbon emissions is prompting a rapid move toward electrified mobility and expanded deployment of solar and wind on the electric grid. If those trends escalate as expected, the need for better methods of storing electrical energy will intensify.

"We need all the strategies we can get to address the threat of climate change," says Elsa Olivetti PhD '07, the Esther and Harold E. Edgerton Associate Professor in Materials Science and Engineering. "Obviously, developing technologies for grid-based storage at a large scale is critical. But for mobile applications—in

Above Solid-state batteries now being developed could be key to achieving the widespread adoption of electric vehicles—potentially a major step toward a carbon-free transportation sector. A team of researchers from MIT and the University of California, Berkeley, has demonstrated the importance of keeping future low-cost, large-scale manufacturing in mind when exploring novel battery concepts. Photo: Zora Zhuang/iStock particular, transportation—much research is focusing on adapting today's lithium-ion battery to make versions that are safer, smaller, and can store more energy for their size and weight."

Traditional lithium-ion batteries continue to improve, but they have limitations that persist, in part because of their structure. A lithium-ion battery consists of two electrodes—one positive and one negative—sandwiched around an organic (carbon-containing) liquid. As the battery is charged and discharged, electrically charged particles (or ions) of lithium pass from one electrode to the other through the liquid electrolyte.

One problem with that design is that at certain voltages and temperatures, the liquid electrolyte can become volatile and catch fire. "Batteries are generally safe under normal usage, but the risk is still there," says Kevin Huang PhD '15, a research scientist in Olivetti's group.

Another problem is that lithium-ion batteries are not well-suited for use in vehicles. Large, heavy battery packs take up space and increase a vehicle's overall weight, reducing fuel efficiency. But it's proving difficult to make today's lithium-ion batteries smaller and lighter while maintaining their energy density, that is, the amount of energy they store per gram of weight.

To solve those problems, researchers are changing key features of the lithium-ion battery to make an all-solid, or "solid-state," version. They replace the liquid electrolyte in the middle with a thin, solid electrolyte that's stable at a wide range of voltages and temperatures. With that solid electrolyte, they use a high-capacity positive electrode and a high-capacity, lithium metal negative electrode that's far thinner than the usual layer of porous carbon. Those changes make it possible to shrink the overall battery considerably while maintaining its energy-storage capacity, thereby achieving a higher energy density.

"Those features—enhanced safety and greater energy density—are probably the two most-often-touted advantages of a potential solid-state battery," says Huang. He then quickly clarifies that "all of these things are prospective, hoped for, and not necessarily realized." Nevertheless, the possibility has many researchers scrambling to find materials and designs that can deliver on that promise.

Thinking beyond the lab

Researchers have come up with many intriguing options that look promising—in the lab. But Olivetti and Huang believe that additional practical considerations may be important, given the urgency of the climate change challenge. "There are always metrics that we researchers use in the lab to evaluate possible materials and processes," says Olivetti. Examples might include energy storage capacity and charge/discharge rate. When performing basic research—which she deems both necessary and important—those metrics are appropriate. "But if the aim is implementation, we suggest adding a few metrics that specifically address the potential for rapid scaling," she says.

Based on industry's experience with current lithium-ion batteries, the MIT researchers and their colleague Gerbrand Ceder, the Daniel M. Tellep Distinguished Professor of Engineering at the University of California, Berkeley, suggest three broad questions that can help identify potential constraints on future scale-up as a result of materials selection. First, with this battery design, could materials availability, supply chains, or price volatility become a problem as production scales up? (Note that the environmental and other concerns raised by expanded mining are outside the scope of this study.) Second, will fabricating batteries from these materials involve difficult manufacturing steps during which parts are likely to fail? And third, do manufacturing measures needed to ensure a high-performance product based on these materials ultimately lower or raise the cost of the batteries produced?

To demonstrate their approach, Olivetti, Ceder, and Huang examined some of the electrolyte chemistries and battery structures now being investigated by researchers. To select their examples, they turned to previous work in which they and their collaborators used text- and data-mining techniques to gather information on materials and processing details reported in the literature. From that database, they selected a few frequently reported options that represent a range of possibilities.

Materials and availability

In the world of solid inorganic electrolytes, there are two main classes of materials—the oxides, which contain oxygen, and the sulfides, which contain sulfur. Olivetti, Ceder, and Huang focused on one promising electrolyte option in each class and examined key elements of concern for each of them.

The sulfide they considered was LGPS, which combines lithium, germanium, phosphorus, and sulfur. Based on availability considerations, they focused on the germanium, an element that raises concerns in part because it's not generally mined on its own. Instead, it's a byproduct produced during the mining of coal and zinc.

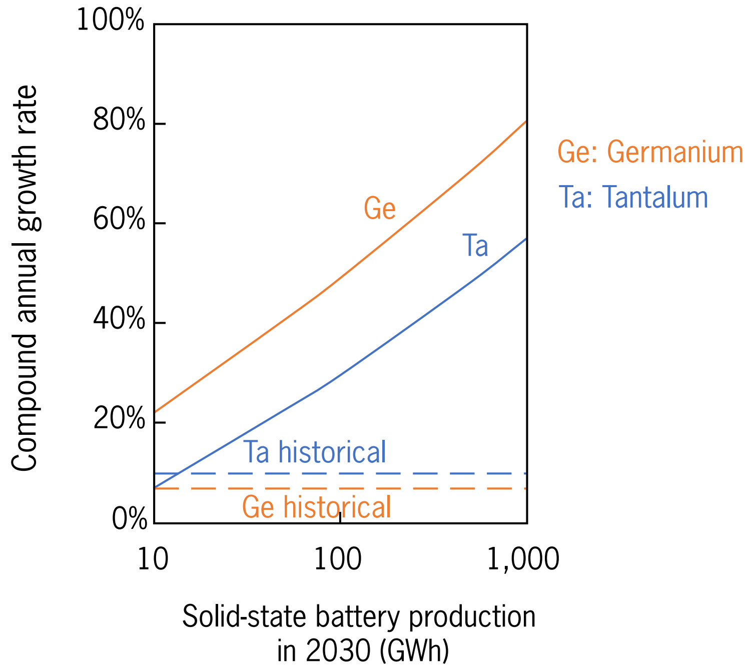
To investigate its availability, the researchers looked at how much germanium was produced annually in the past six decades during coal and zinc mining and then at how much could have been produced. The outcome suggested that 100 times more germanium could have been produced, even in recent years. Given that supply potential, the availability of germanium is not likely to constrain the scale-up of a solid-state battery based on an LGPS electrolyte.

The situation looked less promising with the researchers' selected oxide, LLZO, which consists of lithium, lanthanum, zirconium, and oxygen. Extraction and processing of lanthanum are largely concentrated in China, and there's limited data available, so the researchers didn't try to analyze its availability. The other three elements are abundantly available. However, in practice, a small quantity of another element—called a dopant—must be added to make LLZO easy to process. So the team focused on tantalum, the most frequently used dopant, as the main element of concern for LLZO.

Tantalum is produced as a byproduct of tin and niobium mining. Historical data show that the amount of tantalum produced during tin and niobium mining was much closer to the potential maximum than was the case with germanium. So the availability of tantalum is more of a concern for the possible scale-up of an LLZO-based battery.

But knowing the availability of an element in the ground doesn't address the steps required to get it to a manufacturer. So the researchers investigated a follow-on question concerning the supply chains for critical elements—mining, processing, refining, shipping, and so on. Assuming that abundant supplies are available, can the supply chains that deliver those materials expand quickly enough to meet the growing demand for batteries?

The figure on this page focuses on how much the supply chains for germanium and tantalum would need to grow to meet projected demand for electric vehicles. The horizontal axis shows solid-state battery production in 2030—not in number of batteries but in the total amount of energy in gigawatt-hours (GWh) that would be needed to power a projected fleet of electric vehicles in 2030, as estimated in several industry reports.



Growth in materials supply chains needed to achieve a given solid-state battery production volume in 2030 (in gigawatt-hours) These curves show the compound annual growth rate (CAGR) of supply chains for two materials needed to meet various production levels of two types of solid-state batteries in 2030. The orange curve shows germanium, which is needed for batteries based on LGPS electrolytes, while the blue curve shows tantalum, a dopant used in making LLZO-based batteries. The horizontal dashed lines show the maximum historical CAGRs for the same two elements.

The vertical axis focuses on the amount of germanium and tantalum required for each level of solid-state battery production in 2030. The curves show the compound annual growth rate (CAGR), so the growth from year to year, needed to supply the germanium (orange) and tantalum (blue) for each level of solid-state battery production. For reference, the horizontal orange and blue dashed lines show the maximum historical CAGRs for germanium and tantalum, respectively.

As an example, an electric vehicle fleet often cited as a goal for 2030 would require production of enough batteries to deliver a total of 100 GWh. To meet that goal using just LGPS batteries, the supply chain for germanium would need to grow by 50% from year to year—a stretch, since the maximum CAGR in the past has been about 7%. Using just LLZO batteries, the supply chain for tantalum would need to grow by about 30%—a CAGR well above the historical high of about 10%.

Those examples demonstrate the importance of considering both materials availability and supply chains when evaluating different solid electrolytes for their scale-up potential. "Even when the quantity of a material available isn't a concern, as is the case with germanium, scaling all the steps in the supply chain to match the future production of electric vehicles may require a growth rate that's literally unprecedented," says Huang.

Materials and processing

In assessing the potential for scale-up of a battery design, another factor to consider is the difficulty of the manufacturing process and how it may impact cost. Fabricating a solid-state battery inevitably involves many steps, and a failure at any step raises the cost of each battery successfully produced. As Huang explains, "You're not shipping those failed batteries; you're throwing them away. But you've still spent money on the materials and time and processing."

As a proxy for manufacturing difficulty, Olivetti, Ceder, and Huang explored the impact of failure rate on overall cost for selected solid-state battery designs in their database. In one example, they focused on the oxide LLZO. LLZO is extremely brittle, and at the high temperatures involved in manufacturing, a large sheet that's thin enough to use in a high-performance solid-state battery is likely to crack or warp.

To determine the impact of such failures on cost, they modeled four key processing steps in assembling LLZO-based batteries. At each step, they calculated cost based on an assumed yield, that is, the fraction of total units that were successfully processed without failing. With the LLZO, the yield was far lower than with the other designs they examined; and, as the yield went down, the cost of each kilowatt-hour (kWh) of battery energy went up significantly. For example, when 5% more units failed during the final cathode heating step, cost increased by about \$30/kWh—a nontrivial change considering that a commonly accepted target cost for such batteries is \$100/kWh. Clearly, manufacturing difficulties can have a profound impact on the viability of a design for large-scale adoption.

Materials and performance

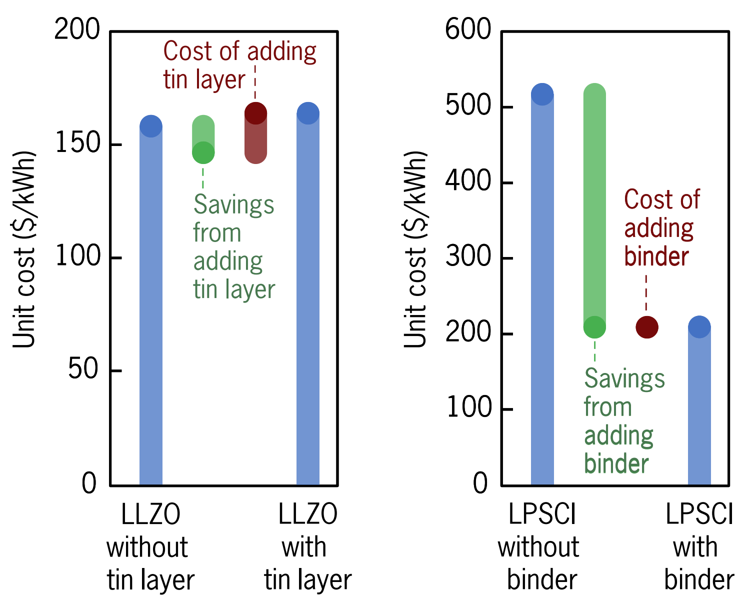
One of the main challenges in designing an all-solid battery comes from "interfaces"—that is, where one component meets another. During manufacturing or operation, materials at those interfaces can become unstable. "Atoms start going places that they shouldn't, and battery performance declines," says Huang.

As a result, much research is devoted to coming up with methods of stabilizing interfaces in different battery designs. Many of the methods proposed do increase performance; and as a result, the cost of the battery in dollars per kWh goes down. But implementing such solutions generally involves added materials and time, increasing the cost per kWh during large-scale manufacturing.

To illustrate that trade-off, the researchers first examined their oxide, LLZO. Here, the goal is to stabilize the interface between the LLZO electrolyte and the negative electrode by inserting a thin layer of tin between the two. The impacts—both positive and negative—on the cost of implementing that solution are shown in the left-hand bar chart below.

The blue bar on the left is the baseline unit cost (in dollars per kWh) of this LLZO-based battery without the layer of tin. The green bar to the right shows the decrease in cost that resulted from the improved performance (noted in the caption). The red bar shows the increase in cost due to the added materials and deposition of the tin layer using a process called sputtering. The right-hand blue bar shows the final cost per kWh, which is higher than the starting cost. So the solution to the instability problem that looked promising in the lab would actually make the battery more, rather than less, expensive during manufacturing.

In another analysis, the researchers looked at a sulfide electrolyte called LPSCl, which consists of lithium, phosphorus, and sulfur with a bit of added chlorine. In this case, the positive electrode incorporates particles of the electrolyte material—a method of ensuring that the lithium ions can find a pathway through the electrolyte to the other electrode. However, the added electrolyte particles are not compatible with other particles in the positive electrode—another interface



Trade-off between battery performance and battery processing cost The left-hand chart shows the cost of manufacturing an LLZO-based battery without and with a thin layer of tin between the negative electrode and the electrolyte. The added tin separator increases capacity by 16 milliamp-hours per gram, which reduces unit cost, as shown by the green bar. However, the cost of including the tin layer—shown by the red bar—exceeds the savings so that the final cost is higher than the original cost. The right-hand chart shows the cost savings resulting from adding a binder material to the positive electrode of an LPSCl solid-state battery. Adding 1% (by weight) of the binder increases capacity by 65 milliamp-hours per gram and brings a \$300 drop in unit cost. Since adding the binder costs almost nothing (the red bar), the full reduction in cost is achieved.

problem. In this case, a standard solution is to add a "binder," another material that makes the particles stick together.

The right-hand chart on page 13 shows the impacts on cost of implementing that solution during manufacturing. The left-hand blue bar is the cost per kWh of manufacturing the LPSCl-based battery without the added binder. As a result of its poor performance, the cost is more than $500/kWh. The green bar shows the impacts of adding the binder. Performance increases significantly, and the cost drops by almost $300/kWh. The red bar represents the cost of adding 1% (by weight) of binder—a cost so low that the red bar is difficult to see. As the right-hand blue bar shows, essentially all of the cost decrease resulting from adding the binder is realized. The method implemented to solve the interface problem pays off in lower costs.

The researchers performed similar studies of other promising solid-state batteries reported in the literature, and their results were consistent: The choice of battery materials and processes can affect not only near-term outcomes in the lab but also the feasibility and cost of manufacturing the proposed solid-state battery at the scale needed to meet future demand. The results also showed that considering all three factors together—availability, processing needs, and battery performance—is important because there may be collective effects and trade-offs involved.

Olivetti is proud of the range of concerns the team's approach can probe. But she stresses that it's not meant to replace traditional metrics used to guide materials and processing choices in the lab. "Instead, it's meant to complement those metrics by also looking broadly at the sorts of things that could get in the way of scaling"—an important consideration given what Huang calls "the urgent ticking clock" of clean energy and climate change.

NOTES

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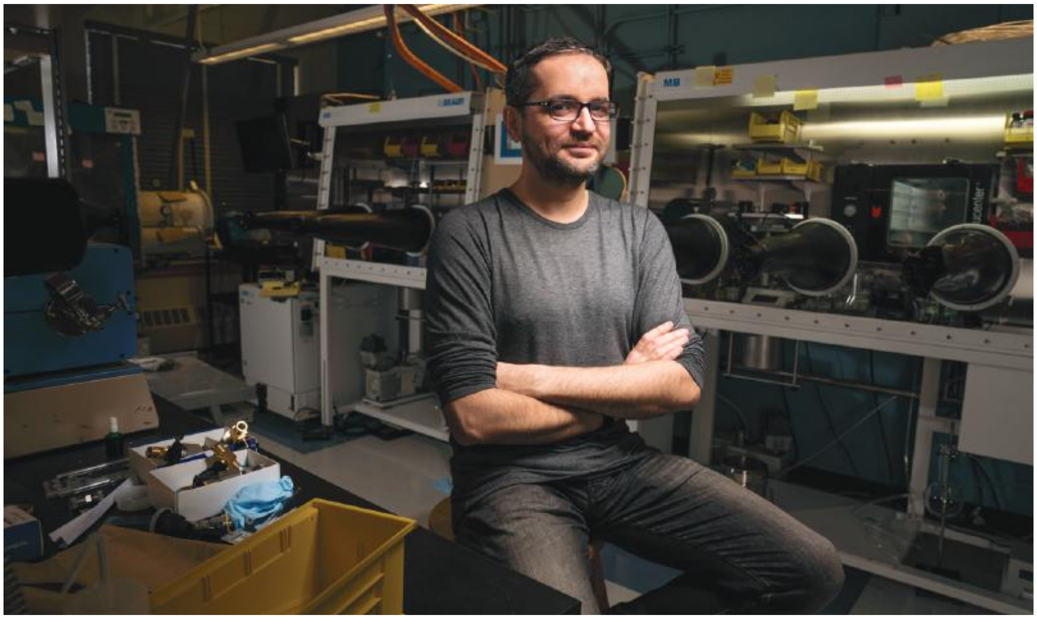
K.J. Huang, G. Ceder, and E.A. Olivetti. "Manufacturing scalability implications of materials choice in inorganic solid-state batteries." *Joule*, vol. 5, issue 3, December 23, 2020. Online: doi.org/10.1016/j.joule.2020.12.001.

R. Mahbub, K. Huang, Z. Jensen, Z.D. Hood, J.L.M. Rupp, and E.A. Olivetti. "Text mining for processing conditions of solid-state battery electrolytes." *Electrochemistry Communications*, vol. 121, December 2020. Online: doi.org/10.1016/j.elecom.2020.106860.



Fine-tuning new materials for energy devices

First look at atomic structure reveals path forward

Nancy W. Stauffer, MITEI

IN BRIEF

An MIT chemist and his international collaborators have announced new insights into a remarkable class of highly porous, crystalline materials called metal-organic frameworks, or MOFs. In rare cases, MOFs can be made electrically conductive, producing materials that could enable significant advances in batteries, fuel cells, catalysts, and more. But it hasn't been clear how to design such MOFs with desired properties or functions. Guided by fundamental studies, the MIT-led researchers were able to grow MOFs as single crystals large enough that a suite of imaging tools could—for the first time—determine their atom-by-atom structure. The researchers could then establish the link between structural details and properties such as electrical conductivity. Based on that information, device designers and others can now select starting materials and synthesis conditions that will produce MOFs optimized for important products and industrial processes.

For more than two decades, much research has focused on a family of materials known as metal-organic frameworks, or MOFs. These special, sponge-like structures are highly porous, have the highest internal surface area of any known material, and generally act as electrical insulators. Moreover, their properties and functions can be altered by changing their composition, their structure, and the conditions under which they are made.

Mircea Dincă, the W.M. Keck Professor of Energy in the Department of Chemistry, has long been intrigued by

Above Studies by Professor Mircea Dincă (pictured) and his collaborators have revealed the atomic-level structure of metal-organic frameworks, or MOFs, a broad family of materials with varying properties. The findings provide design principles for developing new MOF materials that may make possible significant advances in a variety of energy-related technologies. Photo: Bryce Vickmark

MOFs and the possibility of designing versions for specific practical uses. In 2015, he and his MIT team developed a way to make MOFs that don't decompose when exposed to moisture and are therefore suited for use in heat pumps, gas separations and storage, and other industrially important processes. Then, in 2017, they demonstrated MOFs—usually considered electrical insulators—that had electrical conductivity high enough that they could be used in practical devices such as supercapacitors for storing large amounts of energy.

The unusual combination of high porosity and excellent conductivity offered by electrically conductive MOFs has opened up potential applications ranging from batteries, supercapacitors, and fuel cells to electrocatalysts and chemical sensors. However, the development of practical devices has been slowed by the difficulty of readily determining the precise crystalline structure of a given MOF.

"In order to be able to make better materials, you first have to understand what their structure is," says Dincă. Only with a clear understanding of the atom-by-atom structure of a material can one figure out what aspects of that structure determine various properties. "It's a fundamental requirement for making better materials."

So far, there hasn't been an easy way to get a clear, atomic-level image of the type of MOF structures that show high electrical conductivity. The reason: Getting an image with sufficient detail typically requires growing single crystals. "But single crystals of these particular MOF materials haven't been large enough to examine using the most common technique, X-ray diffraction imaging," explains Dincă. "Imaging them with the necessary atomic precision has required using electron diffraction, and not many labs have that capability."

Back when they first measured high electrical conductivity in their MOFs, Dincă and his team set out to grow MOF crystals large enough to use X-ray diffraction to get the atomic-level information they needed. But that, says Dincă, turned out to be very difficult.

The growth habits of MOFs

The challenge in growing large MOF crystals stems from how the crystals like to grow. A single building block of a MOF is a core made of metal ions (electrically charged particles) surrounded by chemically bound arms, or "ligands," made of organic (carbon-containing) molecules that radiate outward. Growth occurs when those individual building blocks link together. They can connect side by side to form flat sheets similar to two-dimensional honeycomb sheets of graphene. And they can grow upward, with the flat sheets piling on top of one another. The result then is a regular array of metal ions connected by ligands, which creates a cage-like structure with open pores. For the final result to be a single crystal, all the linkages must occur without any mistakes. A single crystal is, by definition, nearly defect-free.

The problem has been that MOFs grow far more readily in the vertical direction than in the horizontal plane. As a result, single crystals tend to be tall and skinny—and not large enough to analyze using common X-ray diffraction techniques. The usual strategy for controlling how crystals grow involves systematically changing reactant concentrations or reaction temperature and time. But those approaches haven't altered the directions in which MOFs grow and have yielded only slightly larger crystals.

Dincă and his collaborators realized that they needed to find a way to control the fundamental mechanisms that lead to different growth rates in different directions. For growth to happen, linkages need to break and re-form; those that break more easily are said to be more reversible. The chemical bonds between the metal ions and the ligands in the horizontal sheets are far stronger than the connections that link the stacked up sheets together. Because they're more reversible, the connections controlling vertical growth break and form at a faster rate than the bonds controlling horizontal growth do. As a result, upward growth exceeds horizontal spreading.

In their earlier work on conducting MOFs, Dincă and his team had focused largely on a single particularly promising ligand molecule. But now they needed to find one with characteristics that would elicit a different growth behavior. For example, they could use a molecule with a different distribution of electrons, that is, exactly where the positive and negative charges occur in its physical structure. "Because plus will attract minus and minus will attract plus, how that distribution occurs within a molecule influences how copies of that molecule will arrange themselves with respect to each other—and that ultimately dictates how the molecules stack up and connect with each other," explains Dincă.

They could also choose a ligand molecule with lower electron density in certain regions, thereby making it more acidic. If the molecule binding with the metal is more acidic, it will more easily lose a proton (a charged hydrogen atom), leaving an oxygen atom to connect to the metal—a chemical bond that is more reversible because it's weaker. That change should encourage growth in the horizontal plane.

Based on theoretical analyses and calculations, the team identified a ligand molecule with those characteristics: hexahydroxy-tetraazanaphthotetraphene, or HHTT. Initial experiments with the HHTT ligand were encouraging: The researchers were able to grow larger single crystals than they could using their previous ligand.

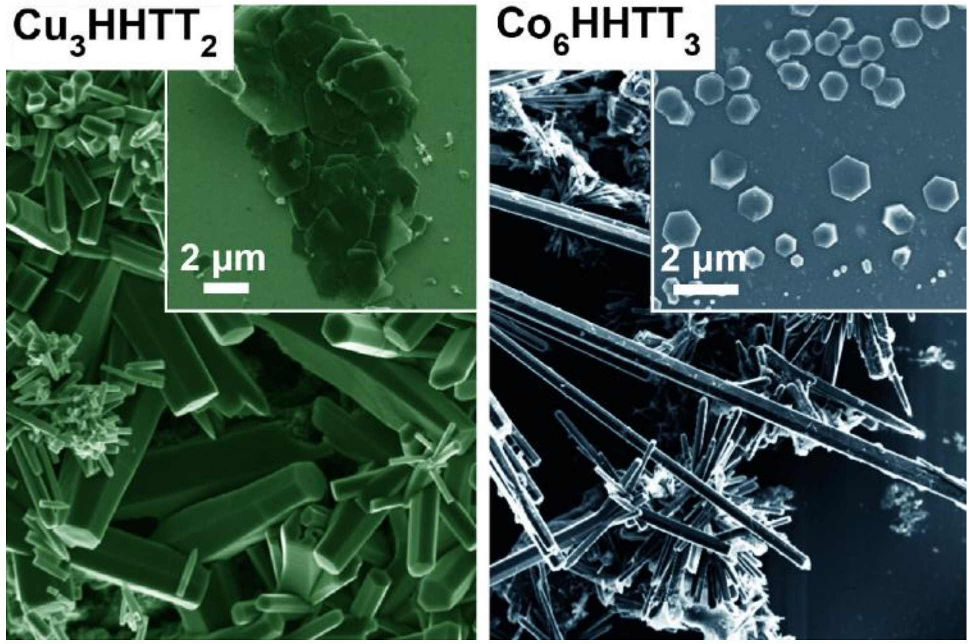
But they could add still one more factor to their MOF design toolkit: They could use different metals with their HHTT ligand. The metal can affect the connections between the stacked layers, thereby changing the rate of vertical growth.

To explore the effect of using different metals, they tried combining the HHTT ligand with cobalt, nickel, copper, and magnesium. The result was MOF materials that were related to one another but had slight structural differences. "Using our diffraction techniques, we could actually tell the very minute differences between all of these materials," says Dincă.

Moreover, they could stabilize the growth to produce and isolate specific single-crystal structures on demand. The images on this page are scanning electron microscopy (SEM) micrographs of single crystals grown using the HHTT ligand. By optimizing the synthesis conditions, the researchers were able to make high-quality, relatively large single crystals of copper-HHTT in the form of plates (left) and of cobalt-HHTT in the form of rods (right).

Dincă notes that each of the rods in the right-hand image is made up of thousands of metal-ligand units that are connected side by side to form hexagonal sheets, which then stack up to form a hexagonal rod, as is evident in the end-on views in the inset image. "That's called crystal morphology," explains Dincă. "The crystal shape often takes on what the molecular shape is." Each rod is about 20 microns in diameter and 200 microns in length—large enough to be characterized using single-crystal X-ray diffraction analysis.

The SEM micrograph provides physical images of the rod-shaped crystals. So their size and hexagonal shape together confirm that the new metal-ligand combination yields both greater horizontal growth and a larger overall crystal size.



Single MOF crystals grown on demand with selected shapes Using a specially selected organic ligand combined with copper or cobalt metal ions, collaborators at MIT and other institutions grew the high-quality single crystals shown in these scanning electron microscope images. By optimizing the synthesis conditions, the researchers could isolate the copper-based crystals as plates (left) and the cobalt-based crystals as rods (right). The hexagonal shape of the rods—visible in the end views in the inset—reflects the hexagonal shape of the individual metal-ligand building blocks. Images courtesy of the researchers and edited by MIT News

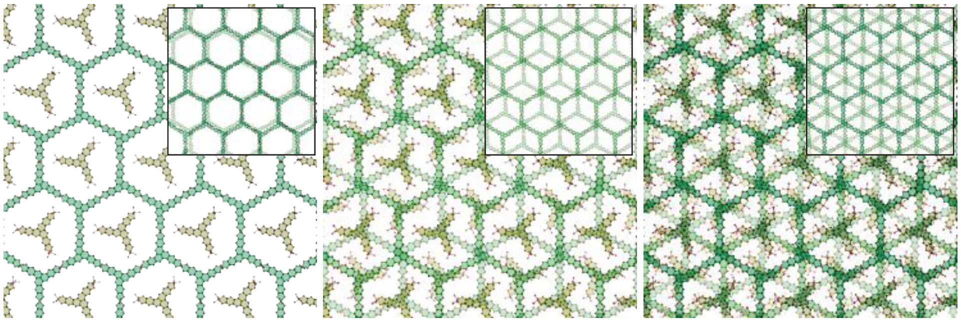
Stacking, slippage, and electrical conductivity

The ability to grow large crystals and examine them using a variety of diffraction techniques creates another opportunity: The researchers could now examine a morphology of interest for controlling electrical conductivity, namely, "slippage" between adjacent layers of their MOF sheets.

The figures on page 18 demonstrate the concept. The illustrations are representations based on X-ray diffraction analysis of a cobalt-HHTT crystal. The views look vertically down at the three-dimensional structure. The left-hand illustration shows the view when looking at only the top layer. If all the layers were stacked in perfect alignment, with the metal-ligand units centered on top of one another, this top layer would eclipse the layers underneath. The view down through all the stacked layers would look like the top layer, including the open pores. However, in this structure, the underneath layers are slid or twisted relative to the top layer, resulting in so-called staggered packing. The middle and right-hand illustrations show the view through two and three layers, respectively. In both cases, the open pores that occur in the top layer are eliminated.

Three-dimensional materials like MOFs can conduct electricity along their horizontal sheets or perpendicular to those sheets. MOFs generally conduct more easily horizontally than vertically. But slippage may alter that tendency—and may offer another way to fine-tune MOFs for particular applications.

To explore that possibility, Dincă and his team fabricated samples using their HHTT ligand and their four metals, producing two versions of each sample—one with eclipsed packing and the other with staggered packing. They then



Stacking arrangement of MOF sheets based on analysis of cobalt-HHTT These illustrations represent the view looking vertically down through the stacked layers that make up this three-dimensional structure. The left-hand image looks only at the top layer. If all the sheets below it were perfectly aligned, they would be eclipsed by this top layer and not be visible. But in this structure, the underneath layers are slid or twisted relative to the top one. As a result, in the view through two or three layers—shown in the middle and right-hand image, respectively—the open pores visible in the top layer are eliminated. The researchers' experimental measurements show that stacking arrangement affects electrical conductivity.

measured the horizontal and vertical conductivity of the eight samples.

They concluded that whether layers were eclipsed or staggered did affect conductivity. For the most part, conductivity in the horizontal plane was higher than it was in the vertical direction in both versions, as expected. But in general, both conductivities—horizontal and vertical—were higher with eclipsed packing than with staggered packing. So the eclipsed packing encouraged electron flow in both directions.

The researchers highlight some other results of note. With the eclipsed version of copper-HHTT, the observed horizontal conductivity compared favorably with the highest conductivity reported in any MOF. And with nickel-HHTT, the eclipsed version was 10 times more conductive than the staggered version. Vertical conductivity was also correlated with closer stacking of the layers. With almost all of their samples, vertical conductivity became higher as the stacked layers got closer together.

"Clearly, determining the kind of slippage you have is very important for understanding overall charge transport," says Dincă. "How positive and negative charges travel along a single plane and jump from one plane to another is very much determined by what the slippage is and by the interlayer distance."

Putting MOFs to work

Dincă and his international team have now established a clear correlation between the structural details and the properties of conductive MOFs. Their methods and results provide other researchers and device designers with guidelines for developing MOFs tailored for specific uses.

But inside Dincă's lab at MIT, the fundamental work continues, with students and postdocs finding ways to grow MOFs for a variety of practical devices. For example, they have demonstrated a new class of microporous electrodes for use in electrical energy storage devices such as batteries and supercapacitors. They are devising new methods for synthesizing and depositing MOF thin films on substrates for possible use as electrocatalysts and for making MOF-based membranes, some specially designed for gas separation—now an energy-intensive process in many industries. They are also designing MOFs with electronic properties that should prove useful in solar energy conversion and light harvesting. And they are making fluorescent MOFs that could detect certain molecules and signal their presence by emitting fluorescent light.

Dincă believes that MOFs are uniquely suited for addressing important societal challenges in transportation, pollution control, energy conversion and storage, and other areas where traditional materials are reaching the limits of their performance. "With MOFs, the possibilities in terms of structure and function are virtually endless," says Dincă. He and his team hope to explore as many of those possibilities as they can.

NOTES

This work was led by MIT Professor Mircea Dincă and involved collaborators from MIT's departments of Chemistry, Biology, and Electrical Engineering and Computer Science; Peking University and the Shanghai Advanced Research University in China; Stockholm University in Sweden; the University of Oregon; and Purdue University. This research was supported by the U.S. Army Research Office and by Automobili Lamborghini. More information can be found in:

J.H. Dou, M.Q. Arguilla, Y. Luo, et al. "Atomically precise single-crystal structures of electrically conducting 2D metal–organic frameworks." *Nature Materials*, vol. 20, pp. 222–228, November 2020. Online: doi.org/10.1038/s41563-020-00847-7.

To boost emissions reductions from electric vehicles, know when to charge

Transportation-related emissions are increasing globally. Currently, light-duty vehicles—namely, passenger cars such as sedans, SUVs, or your parents' minivans—contribute about 20% of the net greenhouse gas emissions in the United States. But studies have shown that switching out your conventional gas-guzzling car for a vehicle powered by electricity can make a significant dent in reducing these emissions.

A study published in *Environmental Science and Technology* takes this a step further by examining how to reduce the emissions associated with the electricity source used to charge an electric vehicle (EV). Taking into account regional charging patterns and the effect of ambient temperature on car fuel economy, researchers at the MIT Energy Initiative (MITEI) find that the time of day when an EV is charged significantly impacts the vehicle's emissions.

The time of day when an electric vehicle (EV) is charged can have a large impact on reducing its emissions. In California, home to half of the electric vehicles in the United States, charging at midday reduces EV emissions by more than 40% when compared to charging at night. Photo: Andrew Roberts/Unsplash

"If you facilitate charging at particular times, you can really boost the emissions reductions that result from growth in renewables and EVs," says Ian Miller SM '18, the lead author of the study and a research specialist at MITEI. "So how do we do this? Time-of-use electricity rates are spreading and can dramatically shift the time of day when EV drivers charge. If we inform policy makers of these large time-of-charging impacts, they can then design electricity rates to discount charging when our power grids are renewable-heavy. In solar-heavy regions, that's midday. In wind-heavy regions, like the Midwest, it's overnight."

According to their research, in solar-heavy California, charging an electric vehicle overnight produces 70% more emissions than charging midday (when more solar energy powers the grid). Meanwhile, in New York, where nuclear and hydro power constitute a larger share of the electricity mix during the night, the best charging time is the opposite. In this region, charging a vehicle overnight actually reduces emissions by 20% relative to daytime charging.

"Charging infrastructure is another big determinant when it comes to facilitating charging at specific times—during the day especially," adds Emre Gençer, co-author and a research scientist at MITEI. "If you need to charge your EV midday, then you need to have enough charging stations at your workplace. Today, most people charge their vehicles in their garages overnight, which is going to produce higher emissions in places where it is best to charge during the day."

In the study, Miller, Gençer, and Maryam Arbabzadeh, a postdoctoral associate at MITEI, make these observations in part by calculating the percentage of error in two common EV emission modeling approaches that ignore hourly variation in the grid and temperature-driven variation in fuel economy. Their results show that the combined error from these standard methods exceeds 10% in 30% of the cases, and reaches 50% in California, which is home to half of the EVs in the United States.

"If you don't model time of charging, and instead assume charging with annual average power, you can misestimate EV emissions," says Arbabzadeh. "To be sure, it's great to get more solar on the grid and more electric vehicles using that grid. No matter when you charge your EV in the U.S., its emissions will be lower than a similar gasoline-powered car; but if EV charging occurs mainly when the sun is down, you won't get as much benefit when it comes to reducing emissions as you think when using an annual average."

Seeking to lessen this margin of error, the researchers use hourly grid data from 2018 and 2019—along with hourly charging, driving, and temperature data—to estimate emissions from EV use in 60 cases across the United States. They then introduce and validate a novel method (with less than 1% margin of error) to accurately estimate EV emissions. They call it the "average day" method.

"We found that you can ignore seasonality in grid emissions and fuel economy and still accurately estimate yearly EV emissions and charging-time impacts," says Miller. "This was a pleasant surprise. In Kansas last year, daily grid emissions rose about 80% between seasons, while EV power demand rose about 50% due to temperature changes. Previous studies speculated that ignoring such seasonal swings would hurt accuracy in EV emissions estimates, but they never actually quantified the error. We did—across diverse grid mixes and climates—and found the error to be negligible."

This finding has useful implications for modeling future EV emissions scenarios. "You can get accuracy without computational complexity," says Arbabzadeh. "With the average-day method, you can accurately estimate EV emissions and charging impacts in a future year without needing to simulate 8,760 values of grid emissions for each hour of the year. All you need is one average-day profile, which means only 24 hourly values, for grid emissions and other key variables. You don't need to know seasonal variance from those average-day profiles."

The researchers demonstrate the utility of the average-day method by conducting a case study in the southeastern United States from 2018 to 2032 to examine how renewable growth in this region may impact future EV emissions. Assuming a conservative grid projection from the U.S. Energy Information Administration, the results show that EV emissions decline only 16% if charging occurs overnight, but more than 50% if charging occurs midday. In 2032, compared to a similar hybrid car, EV emissions per mile are 30% lower if charged overnight, and 65% lower if charged midday.

The model used in this study is one module in a larger modeling program called the Sustainable Energy Systems Analysis Modeling Environment (SESAME). This tool, developed at MITEI, takes a systems-level approach to assess the complete carbon footprint of today's evolving global energy system.

"The idea behind SESAME is to make better decisions for decarbonization and to understand the energy transition from a systems perspective," says Gençer. "One of the key elements of SESAME is how you can connect different sectors together—'sector coupling'—and in this study, we are seeing a very interesting example from the transportation and electric power sectors. Right now, as we've been claiming, it's impossible to treat these two sector systems independently, and this is a clear demonstration of why MITEI's new modeling approach is really important, as well as how we can tackle some of these impending issues."

In ongoing and future research, the team is expanding its charging analysis from individual vehicles to whole fleets of passenger cars in order to develop fleet-level decarbonization strategies. This work seeks to answer questions such as how California's proposed ban of gasoline car sales in 2035 would impact transportation emissions. The researchers are also exploring what fleet electrification could mean—not only for greenhouse gases, but also for the demand for natural resources such as cobalt—and whether EV batteries could provide significant grid energy storage.

"To mitigate climate change, we need to decarbonize both the transportation and electric power sectors," says Gençer. "We can electrify transportation, and it will significantly reduce emissions, but what this paper shows is how you can do it more effectively."

Kelley Travers, MITEI

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This research was sponsored by ExxonMobil Research and Engineering through the MIT Energy Initiative Low-Carbon Energy Centers. For more information, see the following:

I. Miller, M. Arbabzadeh, and E. Gençer. "Hourly power grid variations, electric vehicle charging patterns, and operating emissions." *Environmental Science and Technology*, vol. 54, no. 24, pp. 16071–16085, November 2020. Online: doi.org/10.1021/acs.est.0c02312.

Concept for a hybrid-electric plane may reduce aviation's air pollution problem

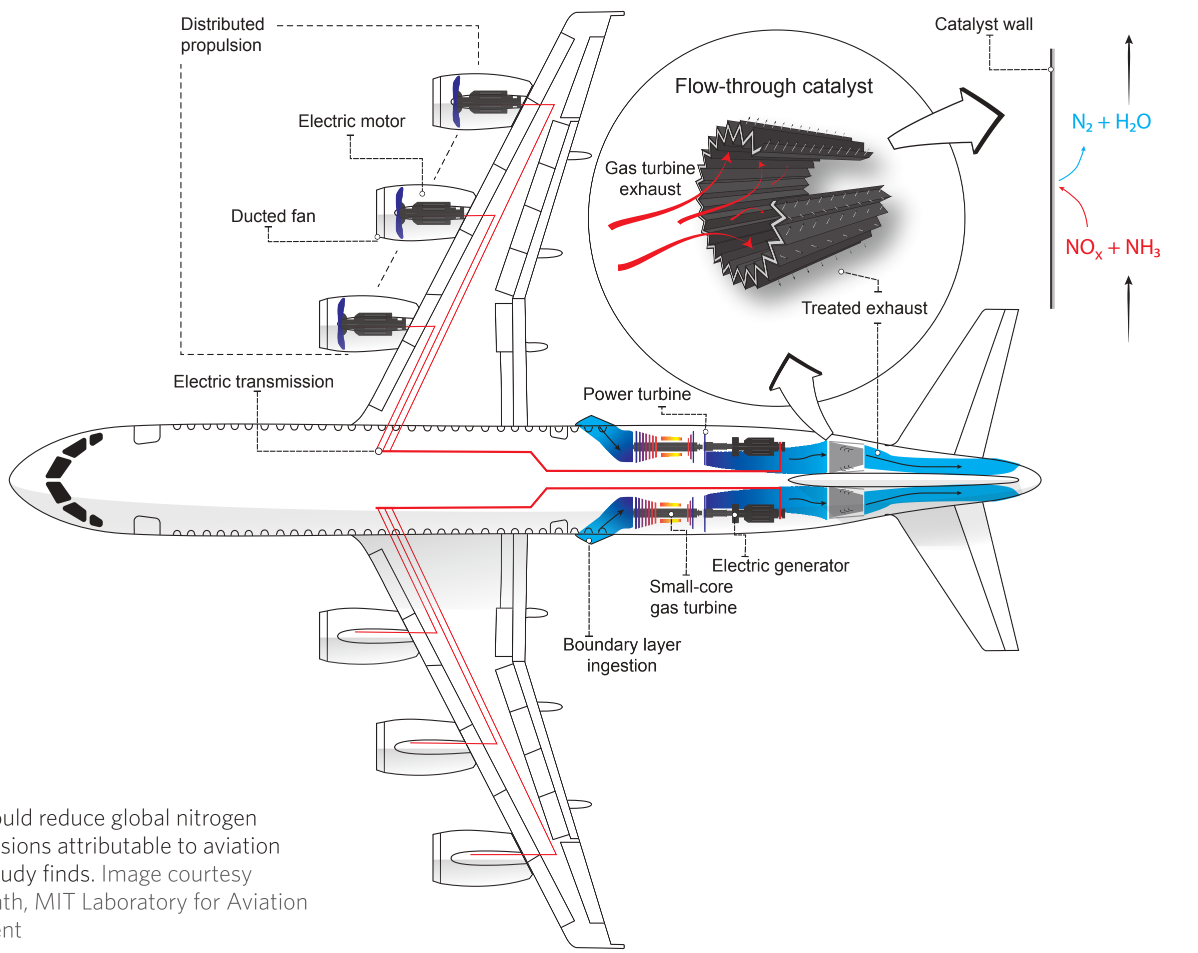
At cruising altitude, airplanes emit a steady stream of nitrogen oxides into the atmosphere, where the chemicals can linger to produce ozone and fine particulates. Nitrogen oxides, or NO_x, are a major source of air pollution and have been associated with asthma, respiratory disease, and cardiovascular disorders. Previous research has shown that the generation of these chemicals due to global aviation results in 16,000 premature deaths each year.

Now MIT engineers have come up with a concept for airplane propulsion that they estimate would eliminate 95% of aviation's NO_x emissions, and thereby reduce the number of associated early deaths by 92%.

The concept is inspired by emissions-control systems used in ground transportation vehicles. Many heavy-duty diesel trucks today house post-combustion emissions-control systems to reduce the NO_x generated by engines. The researchers now propose a similar design for aviation, with an electric twist.

Today's planes are propelled by jet engines anchored beneath each wing. Each engine houses a gas turbine that powers a propeller to move the plane through the air as exhaust from the turbine flows out the back. Due to this configuration, it has not been possible to use emissions-control devices, as they would interfere with the thrust produced by the engines.

In the new hybrid-electric—or more specifically "turboelectric"—design, a plane's source of power would still be a conventional gas turbine, but it would be integrated within the plane's fuselage (where part of the cargo hold is in current aircraft). Rather than directly powering propellers or fans, the gas turbine would drive a generator, also in the hold, to produce electricity, which would then electrically power the plane's wing-mounted, electrically driven propellers or fans. The emissions produced by the gas turbine would be fed into an emissions-control system, broadly similar to those in diesel vehicles, which would clean the exhaust before ejecting it into the atmosphere.



This new design could reduce global nitrogen oxides (NO_x) emissions attributable to aviation by 95%, an MIT study finds. Image courtesy of Prakash Prashanth, MIT Laboratory for Aviation and the Environment

"This would still be a tremendous engineering challenge, but there aren't fundamental physics limitations," says Steven Barrett, professor of aeronautics and astronautics at MIT. "If you want to get to a net-zero aviation sector, this is a potential way of solving the air pollution part of it, which is significant, and in a way that's technologically quite viable."

The details of the design, including analyses of its potential fuel cost and health impacts, were published in the journal *Energy and Environmental Science*. The paper's co-authors are Prakash Prashanth, Raymond Speth, Sebastian Eastham, and Jayant Sabnis, all members of MIT's Laboratory for Aviation and the Environment.

A semi-electrified plan

The seeds for the team's hybrid-electric plane grew out of Barrett and his team's work investigating the Volkswagen diesel emissions scandal. In 2015, environmental regulators discovered that the car manufacturer had been intentionally manipulating diesel engines to activate onboard emissions-control systems only during lab testing, such that they appeared to meet NO_x emissions standards but in fact emitted up to 40 times more NO_x in real-world driving conditions.

As he looked into the health impacts of the emissions cheat, Barrett also became familiar with diesel vehicles' emissions-control systems in general. Around the same time, he was also looking into the possibility of engineering large, all-electric aircraft.

"The research that's been done in the last few years shows you could probably electrify smaller aircraft, but for big aircraft, it won't happen anytime soon without pretty major breakthroughs in battery technology," Barrett says. "So I thought, maybe we can take the electric propulsion part from electric aircraft, and the gas turbines that have been around for a long time and are super reliable and very efficient, and combine that with the emissions-control technology that's used in automotive and ground power to at least enable semi-electrified planes."

Flying with zero impact

Before airplane electrification had been seriously considered, it might have been possible to implement a concept such as this, for example as an add-on to the back of jet engines. But this design, Barrett notes, would "kill any stream of thrust" that a jet engine would produce, effectively grounding the design.

Barrett's concept gets around this limitation by separating the thrust-producing propellers or fans from the power-generating gas turbine. The propellers or fans would instead be directly powered by an electric generator, which in turn would be powered by the gas turbine. The exhaust from the gas turbine would be fed into an emissions-control system, which could be folded up, accordion-style, in the plane's cargo hold—completely isolated from the thrust-producing propellers.

He envisions the bulk of the hybrid-electric system—gas turbine, electric generator, and emissions-control system—would fit within the belly of a plane, where there can be ample space in many commercial aircraft.

In their paper, the researchers calculate that if such an emissions-control system were implemented on a future hybrid-electric aircraft similar in size to a Boeing 737 or Airbus A320, the extra weight of the emissions-control system and the associated losses would require about 0.6% more fuel to fly a typical route than the hybrid-electric aircraft without the emissions-control system.

"This would be many, many times more feasible than what has been proposed for all-electric aircraft," Barrett says. "This design would add some hundreds of kilograms to a plane, as opposed to adding many tons of batteries, which would be over a magnitude of extra weight."

The researchers also calculated the emissions that would be produced by a large aircraft, with and without an emissions-control system, and found that the hybrid-electric design would eliminate 95% of NO_x emissions.

If this system were rolled out across all aircraft around the world, they further estimate that 92% of pollution-related deaths due to aviation would be avoided. They arrived at this estimate by using a global model to map the flow of aviation emissions through the atmosphere and calculated how much various populations around the world would be exposed to these emissions. They then converted these exposures to mortalities, or estimates of the number of people who would die prematurely as a result of exposure to aviation emissions.

The team is now working on designs for a "zero-impact" airplane that flies without emitting NO_x and other chemicals like climate-altering carbon dioxide.

"We need to get to essentially zero net-climate impacts and zero deaths from air pollution," Barrett says. "This current design would effectively eliminate aviation's air pollution problem. We're now working on the climate impact part of it."

Jennifer Chu, MIT News Office

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Adapted and reprinted with permission of MIT News (news.mit.edu). Further information on this research can be found in:

P. Prashanth, R.L. Speth, S.D. Eastham, J.S. Sabnis, and S.R.H. Barrett. "Post-combustion emissions control in aero-gas turbine engines." *Energy & Environmental Science*, issue 2, 2021. Online: doi.org/10.1039/D0EE02362K.

How can you reduce the environmental impact of your next virtual meeting?

Before you scramble to clean your room or attempt to make your pajamas look a bit less like pajamas, here is a good excuse to keep your video off during your next virtual meeting: reducing your environmental impact. A recent study shows that if you turn your camera off during a videoconference, you can reduce your environmental footprint in that meeting by 96%.

Conducted by a team from MIT, Purdue University, and Yale University, the study uncovers the impacts that internet use has on the environment. This is especially significant considering that many countries have reported at least a 20% increase in internet use since March 2020 due to the Covid-19 lockdowns.

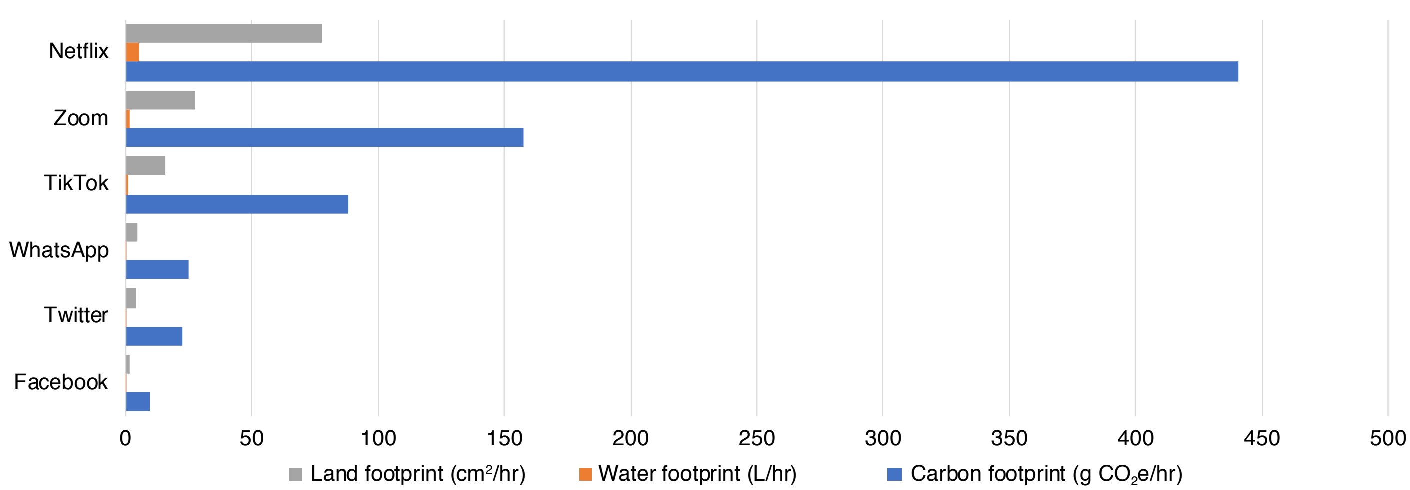
While the shift to a more digital world has made an impressive dent in global emissions overall—thanks in large part to the likely temporary emissions reductions associated with travel—the impact of our increasingly virtual lifestyles should not be overlooked. "The goal of this paper is to raise awareness," says Maryam Arbabzadeh, a postdoctoral associate at the MIT Energy Initiative and a co-author of the study. "It is great that we are reducing emissions in some sectors; but at the same time, using the internet also has an environmental impact contributing to the aggregate. The electricity used to power the internet, with its associated carbon, water, and land footprints, isn't the only thing impacting the environment; the transmission and storage of data also requires water to cool the systems within the data centers."

One hour of streaming or videoconferencing can emit between 150 and 1,000 grams of carbon dioxide, depending on the service. (By comparison, a car produces about 8,887 grams from burning one gallon of gasoline.) That hour also requires two to 12 liters of water and a land area about the size of an iPad Mini. Those hours add up in our daily lives with all the time we're spending on video—and so does the associated environmental footprint.

According to the researchers, if remote work continues through the end of 2021, the global carbon footprint could grow by 34.3 million tons in greenhouse gas emissions. To give a sense of the scale: This increase in emissions would require a forest twice the size of Portugal to fully sequester it all. Meanwhile, the associated water footprint would be enough to fill more than 300,000 Olympic-sized swimming pools, and the land footprint would be equal to roughly the size of Los Angeles.

To store and transmit all of the data powering the internet, data centers consume enough electricity to account for 1% of global energy demand—which is more than the total consumption for many countries. Even before the pandemic, the internet's carbon footprint had been increasing and accounted for about 3.7% of global greenhouse gas emissions.

While there have been studies evaluating the carbon footprint of internet data transmission, storage, and use, the associated water and land footprints have been largely overlooked. To address this gap, the researchers in this study analyze the three major environmental



What is the environmental footprint of your app? Researchers estimate the environmental footprints associated with each gigabyte of data used in common online applications and activities. Their study shows that video streaming makes a significant contribution to the impact of internet use on the environment.

footprints—water, land, and carbon—as they pertain to internet use and infrastructure, providing a more holistic look at environmental impact.

Using publicly available data, the researchers give a rough estimate of the carbon, water, and land footprints associated with each gigabyte of data used in common online apps such as Netflix, Instagram, TikTok, Zoom, and 14 other platforms, as well as general web surfing and online gaming. They find that the more video used, the higher the footprints.

A common streaming service, like Netflix or Hulu, requires 7 gigabytes per hour of high-quality video streaming, translating to an average of 441 g CO_2e (carbon dioxide equivalent) per hour. If someone is streaming for four hours a day at this quality for a month, the emissions rise to 53 kg CO_2e. However, if that person were to instead stream in standard definition, the monthly footprint would only be 2.5 kg CO_2e. That decision would save emissions equivalent to driving a car from Baltimore to Philadelphia, about 93 miles.

Now multiply these savings across 70 million users all streaming in standard definition rather than high definition. That behavioral change would result in a decrease of 3.5 million tons of CO_2e—equating to the elimination of 1.7 million tons of coal, which is about 6% of the total monthly consumption of coal in the United States.

"Banking systems tell you the positive environmental impact of going paperless, but no one tells you the benefit of turning off your camera or reducing your streaming quality. So without your consent, these platforms are increasing your environmental footprint," says Kaveh Madani, who led and directed this study while a visiting fellow at the Yale MacMillan Center.

While many service providers and data centers have been working to improve operation efficiency and reduce their carbon footprints by diversifying their energy portfolios, measures still need to be taken to reduce the footprint of the product. A streaming service's video quality is one of the largest determinants of its environmental footprint. Currently, the default for many services is high-definition, putting the onus on users to reduce the quality of their video in order to improve their footprint. Not many people will be interested in reducing their video quality, especially if the benefits of this action are not well known.

"We need companies to give users the opportunity to make informed, sustainable choices," says Arbabzadeh. "Companies could change their default actions to lead to less environmental impact, such as setting video quality to standard definition and allowing users to upgrade to high definition. This will also require policy makers to be involved—enacting regulations and requiring transparency about the environmental footprint of digital products to encourage both companies and users to make these changes."

The researchers also look at specific countries to understand how different energy systems impact the environmental footprints for an average unit of energy used in data processing and transmission. The data show wide variation in carbon, land, and water intensity. In the United States, where natural gas and coal make up the largest share of electricity generation, the carbon footprint is 9% higher than the world median, but the water footprint is 45% lower and the land footprint is 58% lower. Meanwhile, in Brazil, where nearly 70% of the electricity comes from hydropower, the median carbon footprint is about 68% lower than the world median. The water footprint, on the other hand, is 210% higher than the world median, and increasing reliance on hydropower at the expense of fragile rainforest ecosystems has other substantial environmental costs.

"All of these sectors are related to each other," says Arbabzadeh. "In data centers where electricity comes from a cleaner source, the emissions will be lower; and if it's coming from fossil fuels, then the impact will be higher."

"Right now, we have virtual meetings all over, and we're spending more of our leisure time than ever streaming video content. There is definitely a paradigm shift," she adds. "With some small behavior changes, like unsubscribing from junk emails or reducing cloud storage, we can have an impact on emissions. It is important that we raise public awareness so that collectively, we can implement meaningful personal and systemic changes to reduce the internet's environmental impact and successfully transition to a low-carbon economy."

Kelley Travers, MITEI

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This study was supported by the MIT Energy Initiative, Purdue Climate Change Research Center, the Purdue Center for the Environment, and the Yale MacMillan Center. For more information, see the following:

R. Obringer, B. Rachunok, D. Maia-Silva, M. Arbabzadeh, R. Nateghi, and K. Madani. "The overlooked environmental footprint of increasing Internet use." *Resources, Conservation and Recycling*, vol. 167, April 2021. Online: doi.org/10.1016/j.resconrec.2020.105389.

Long-duration energy storage: Its role and value in securing a carbon-free electric grid

"The overall question for me is how to decarbonize society in the most affordable way," says Nestor Sepulveda SM '16, PhD '20. As a postdoctoral associate at MIT and a researcher with the MIT Energy Initiative (MITEI), he worked with a team over several years to investigate what mix of energy sources might best accomplish this goal. The group's initial studies suggested the "need to develop energy storage technologies that can be cost-effectively deployed for much longer durations than lithium-ion batteries," says Dharik Mallapragada, a research scientist with MITEI.

MIT researchers explore different scenarios and variables to find parameter combinations that would enable innovative, low-cost, long-duration energy storage to potentially make a large impact in a more affordable and reliable energy transition. Photo illustration: Bumper DeJesus, Andlinger Center for Energy and the Environment, Princeton University

In a paper published in *Nature Energy*, Sepulveda, Mallapragada, and colleagues from MIT and Princeton University offer a comprehensive cost and performance evaluation of the role of long-duration energy storage (LDES) technologies in transforming energy systems. LDES, a term that covers a class of diverse, emerging technologies, can respond to the variable output of renewables, discharging electrons for days and even weeks, providing resilience to an electric grid poised to deploy solar and wind power on a large scale.

"If we want to rely overwhelmingly on wind and solar power for electricity—increasingly the most affordable way to decrease carbon emissions—we have to deal with their intermittency," says Jesse Jenkins SM '14, PhD '18, an assistant professor of mechanical and aerospace engineering and the Andlinger Center for Energy and the Environment at Princeton University and former researcher at MITEI.

For their paper, the researchers analyzed whether LDES paired with renewable energy sources and short-duration energy storage options like lithium-ion batteries could indeed power a massive and cost-effective transition to a decarbonized grid. They also investigated whether LDES might even eliminate the need for available-on-demand, or firm, low-carbon energy sources such as nuclear power and natural gas with carbon capture and sequestration.

"The message here is that innovative and low-cost LDES technologies could potentially have a big impact, making a deeply decarbonized electricity system more affordable and reliable," says lead author Sepulveda, who now works as a consultant with McKinsey & Company. But, he notes, "We will still be better off retaining firm low-carbon energy sources among our options."

In addition to Jenkins and Mallapragada, the paper's co-authors include Aurora Edington SM '19, a MITEI research assistant at the time of this research and now a consultant at The Cadmus Group; and Richard K. Lester, the Japan Steel Industry Professor and associate provost at MIT, and former head of the Department of Nuclear Science and Engineering.

"As the world begins to focus more seriously on how to achieve deep decarbonization goals in the coming decades, the insights from these system-level studies are essential," says Lester. "Researchers, innovators, investors, and policy makers will all benefit from knowledge of the cost and technical performance targets that are suggested by this work."

Performance and cost

The team set out to assess the impacts of LDES solutions in hypothetical electric systems that reflect real-world conditions, where technologies are scrutinized not merely by their stand-alone attributes, but by their relative value when matched against other energy sources.

"We need to decarbonize at an affordable cost to society, and we wanted to know if LDES can increase our probability of success while also reducing overall system cost, given the other technologies competing in the space," says Sepulveda.

In pursuit of this goal, the team deployed an electricity system capacity expansion model, GenX, earlier developed by Jenkins and Sepulveda while at MIT. This simulation tool made it possible to evaluate the potential system impact of utilizing LDES technologies, including technologies currently being developed and others that could potentially be developed, for different future low-carbon electric grid scenarios characterized by cost and performance attributes of renewable generation, different types of firm generation, as well as alternative electricity demand projections. The study, says Jenkins, was "the first extensive use of this sort of experimental method of applying wide-scale parametric uncertainty and long-term, systems-level analysis to evaluate and identify target goals regarding cost and performance for emerging long-duration energy storage technologies."

For their study, the researchers surveyed a range of long-duration technologies—some backed by the U.S. Department of Energy's Advanced Research Projects Agency–Energy (ARPA-E) program—to define the plausible cost and performance attributes of future LDES systems based on key parameters that encompass a range of mechanical, chemical, electrochemical, and thermal approaches. These parameters include pumped hydropower storage, vanadium redox flow batteries, aqueous sulfur flow batteries, and firebrick resistance-heated thermal storage, among others.

"Think of a bathtub, where the parameter of energy storage capacity is analogous to the volume of the tub," explains Jenkins. Continuing the analogy, another important parameter, charge power capacity, is the size of the faucet filling the tub, and discharge power capacity is the size of the drain. In the most generalized version of an LDES technology, each attribute of the system can be independently sized. In optimizing an energy system where LDES technology functions as "an economically attractive contributor to a lower-cost, carbon-free grid," says Jenkins, the researchers found that the parameter that matters the most is energy storage capacity cost.

"For a comprehensive assessment of LDES technology design and its economic value to decarbonized grids, we evaluated nearly 18,000 distinctive cases," Edington explains, "spanning variations in load and renewable resource availability, northern and southern latitude climates, different combinations of LDES technologies and LDES design parameters, and choice of competing firm low-carbon generation resources."

Some of the key takeaways from the researchers' rigorous analysis:

- LDES technologies can offer more than a 10% reduction in the costs of deeply decarbonized electricity systems if the storage energy capacity cost (the cost to increase the size of the bathtub) remains under the threshold of $20/kilowatt-hour (kWh). This value could increase to 40% if energy capacity cost of future technologies is reduced to $1/kWh and to as much as 50% for the best combinations of parameters modeled in the space. For purposes of comparison, the current storage energy capacity cost of batteries is around $200/kWh.

- Given today's prevailing electricity demand patterns, the LDES energy capacity cost must fall below $10/kWh to replace nuclear power; for LDES to replace all firm power options entirely, the cost must fall below $1/kWh.

- In scenarios with extensive electrification of transportation and other end uses to meet economywide deep decarbonization goals, it will be more challenging in northern latitudes to displace firm generation under any likely future combination of costs and efficiency performance range for known LDES technologies. This is primarily due to greater peak electricity demand resulting from heating needs in colder climates.

Actionable insights

While breakthroughs in fusion energy, next-generation nuclear power, or carbon capture could well shake up their models, the researchers believe that insights from their study can make an impact right now.

"People working with LDES can see where their technology fits into the future electricity mix and ask: Does it make economic sense from a system perspective?" says Mallapragada. "And it's a call for action in policy and investment in innovation, because we show where the technology gaps lie and where we see the greatest value for research breakthroughs in LDES technology development."

Not all LDES technologies can clear the bar in this design space, nor can there be reliance on LDES as the exclusive means to expand wind and solar swiftly in the near term, or to enable a complete transition to a zero-carbon economy by 2050.

"We show how promising LDES technologies could be," says Sepulveda. "But we also show that these technologies are not the one solution, and that we are still better off with them complementing firm resources."

Jenkins spies niche market opportunities for LDES immediately in places with a lot of wind and solar deployed and limits on transmission to export that power. In such locations, storage could fill up when transmission is at its limit, and export power later while maximizing use of the power line capacity. But LDES technologies must be ready to make a major impact by the late 2030s and 2040s, he believes, by which time economies might need to be weaned off natural gas dependency if decarbonization is to succeed.

"We must develop and deploy LDES and improve other low-carbon technologies this decade, so we can present real alternatives to policy makers and power system operators," he says.

In light of this urgent need, Jenkins at Princeton and Mallapragada at MIT are now working to evaluate and advance technologies with the greatest potential in the storage and energy fields to hasten the zero-carbon goal. With help from ARPA-E and MITEI, they are making the state-of-the-art GenX electricity system planning model an open-source tool for public use as well. If their research and modeling approach can show developers and policy makers what kinds of designs are most impactful, says Sepulveda, "We could have a decarbonized system that's less expensive than today's system if we do things right."

Leda Zimmerman, MITEI correspondent

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This research was supported by a grant from the National Science Foundation, and by the MIT Energy Initiative's Low-Carbon Energy Center for Electric Power Systems. More information can be found in:

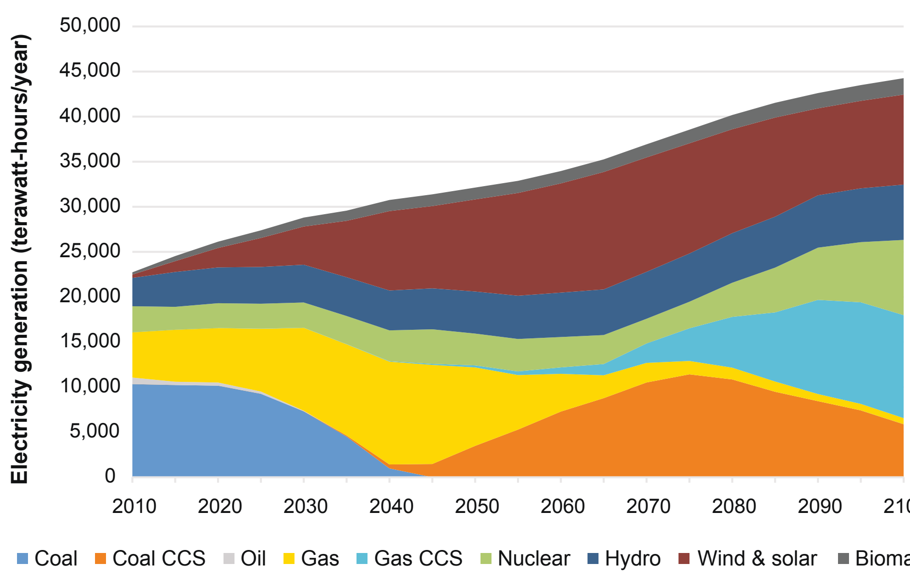
N.A. Sepulveda, J.D. Jenkins, A. Edington, D. Mallapragada, and R.K. Lester. "The design space for long-duration energy storage in decarbonized power systems." *Nature Energy*, March 2021. Online: doi.org/10.1038/s41560-021-00796-8.

Powering through the coming energy transition: Carbon capture and storage is key to achieving climate goals

Aiming to avoid the worst effects of climate change, from severe droughts to extreme coastal flooding, the nearly 200 nations that signed the Paris Agreement set a long-term goal of keeping global warming well below 2 degrees Celsius. Achieving that goal will require dramatic reductions in greenhouse gas emissions, primarily through a global transition to low-carbon energy technologies. In the power sector, these include solar, wind, biomass, nuclear, and carbon capture and storage (CCS). According to more than half of the models cited in the Intergovernmental Panel on Climate Change's (IPCC) Fifth Assessment Report, CCS will be required to realize the Paris goal, but to what extent will it need to be deployed to ensure that outcome?

A study in *Climate Change Economics* led by the MIT Joint Program on the Science and Policy of Global Change projects the likely role of CCS in the power sector in a portfolio of low-carbon technologies. Using the Joint Program's multi-region, multi-sector energy-economic modeling framework to quantify the economic and technological competition among low-carbon technologies as well as the impact of technology transfers between countries, the study assessed the potential of CCS and its competitors in mitigating carbon emissions in the power sector under a policy scenario aligned with the 2°C Paris goal.

The researchers found that under this scenario and the model's baseline estimates of technology costs and performance, CCS will likely be incorporated in nearly 40% of global electricity production by 2100—



The role of carbon capture and sequestration (CCS) in future electricity generation Under a policy scenario designed to achieve the 2°C Paris Agreement goal, CCS is projected to play a major role in the global electricity mix, particularly in the second half of the century. By 2100, plants with CCS could be responsible for nearly 40% of world electricity production, with a third of that production from coal with CCS and the other two-thirds from gas with CCS.

one-third in coal-fired power plants and two-thirds in those run on natural gas (see the figure on page 27).

"Our projections show that CCS can play a major role in the second half of this century in mitigating carbon emissions in the power sector," says Jennifer Morris SM '09, PhD '13, a research scientist in the Joint Program and the MIT Energy Initiative and the lead author of the study. "But in order for CCS to be well-positioned to provide stable and reliable power during that time frame, research and development will need to be scaled up."

That would require a considerable expansion of today's nearly four dozen commercial-scale carbon capture projects around the globe, about half of which are in development.

The study also found that the extent of CCS deployment, especially coal CCS, depends on the assumed fraction of carbon captured in CCS power plants. Under a stringent climate policy with high carbon prices, the penalty on uncaptured emissions can make CCS technologies uneconomical and hinder their expansion. Adding options for higher capture rates or offsetting uncaptured emissions (e.g., by co-firing with biomass, which has already captured carbon through its cultivation and so would produce net negative emissions when combusted) can lead to greater deployment of CCS.

According to the study, CCS deployment will likely vary on a regional basis, with the United States and Europe depending primarily on gas CCS, China on coal CCS, and India embracing both options. Comparing projections of demands for CCS to an assessment of the planet's capacity to store carbon dioxide (CO_2), the authors found that CO_2 storage potential is larger than storage demand at both global and regional scales.

Finally, in evaluating the comparative costs of competing low-carbon technologies, the study found that nuclear generation, if public acceptance and economic issues are resolved, could substitute for CCS in providing clean dispatchable power. Wind and solar could also outcompete CCS, depending on how the costs of intermittency (e.g., systems that keep the lights on when the sun doesn't shine or the wind doesn't blow) are defined. Progress in resolving technical and economic challenges related to intermittency could reduce the need for accelerated CCS deployment.

Ultimately, the authors determined that the power sector will continue to rely on a mix of technological options, and the conditions that favor a particular mix of technologies differ by region.

"This suggests that policy makers should not pick a winner, but rather create an environment where all technologies compete on an economic basis," says Sergey Paltsev, deputy director of the Joint Program and a co-author of the study. "CCS has great potential to be a competitive option, and that potential can increase with additional research and development related to capture rates, CO_2 transport and storage, and applications of CCS technologies to areas outside of power generation."

To that end, Joint Program researchers are pursuing an in-depth analysis of the options and costs for the transportation and long-term storage of CO_2 emissions captured by CCS technology. They are also assessing the potential of CCS in hard-to-abate economic sectors such cement, iron and steel, and fertilizer production.

Mark Dwortzan, MIT Joint Program on the Science and Policy of Global Change

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J. Morris, H. Kheshgi, S. Paltsev, and H. Herzog. "Scenarios for the deployment of carbon capture and storage in the power sector in a portfolio of mitigation options." *Climate Change Economics*, November 2020. Online: doi.org/10.1142/S2010007821500019.

MITEI researchers build supply chain model to support hydrogen economy

Over the past decades, the need for carbon-free energy has driven increasing interest in hydrogen as an environmentally clean fuel. But shifting the economy away from fossils fuels to clean-burning hydrogen will require significant adjustments in current supply chains. To facilitate this transition, an MIT-led team of researchers has developed a new hydrogen supply chain planning model.

"We propose flexible scheduling for trucks and pipelines, allowing them to serve as both storage and transmission," says Guannan He, a postdoctoral associate at the MIT Energy Initiative (MITEI) and lead author of a paper published by *IEEE Transactions on Sustainable Energy* in March. "This is very important to green hydrogen produced from intermittent renewables, because this can provide extra flexibility to meet variability in supply and demand."

Hydrogen has been widely recognized as a promising path to decarbonizing many sectors of the economy because it packs in more energy by weight than even gasoline or natural gas, yet generates zero emissions when used as an energy source. Producing hydrogen, however, can generate significant emissions. According to the U.S. Office of Energy Efficiency and Renewable Energy, 95% of the hydrogen produced today is generated through steam methane reforming (SMR), an energy-intensive process in which methane reacts with water to produce hydrogen and carbon monoxide. A secondary part of this process adds steam to the cooled gas to convert carbon monoxide to carbon dioxide (CO_2) and produce more hydrogen.

Ultimately, hydrogen production today accounts for about 4% of CO_2 emissions globally, says He, and that number will rise significantly if hydrogen becomes popular as a fuel for electric vehicles and such industrial processes as steel refining and ammonia production. Realizing the vision of creating an entirely decarbonized hydrogen economy therefore depends on using renewable energy to produce hydrogen, a task often accomplished through electrolysis, a process that extracts hydrogen from water electrochemically.

However, using renewable energy requires storage to move energy from times and places with peak generation to those with peak demand. And, storage is expensive.

The researchers expanded their thinking about storage to address this key concern: They used trucks in their model both as a means of fuel transmission and of storage—since hydrogen can be readily stored in idled trucks. This tactic reduces costs in the hydrogen supply chain by about 9% by bringing down the need for other storage solutions, says He. "We found it very important to use the trucks in this way," says He. "It can reduce the cost of the system and encourage renewable-based hydrogen production, instead of gas-based production."

Developing the model

Previous studies have attempted to assess the potential benefit of hydrogen storage in power systems, but they have not considered infrastructure investment needs from the perspective of a whole hydrogen supply chain, He says. And such work is critical to enabling a hydrogen economy.

For the new model, the research team—He; MITEI research scientists Emre Gençer and Dharik Mallapragada; Abhishek Bose, an MIT master's student in technology and policy; and Clara F. Heuberger, a researcher at Shell Global Solutions International B.V.—adopted the perspective of a central planner interested in minimizing system costs and maximizing societal benefit. The researchers looked at costs associated with the four main steps in the hydrogen supply chain: production, storage, compression, and transmission. "Unless we take a wholistic approach to analyzing the entire supply chain, it is hard to determine the prospects for hydrogen. This work fills that gap in the literature," Gençer says.

To ensure their model was as comprehensive as possible, the researchers included a wide range of hydrogen-related technologies, including SMR with and without carbon capture and storage, hydrogen transport as a gas or liquid, and transmission via pipeline and trucks. "We have developed a scalable modeling and decision-making tool for a hydrogen supply chain that fully captures the flexibility of various resources as well as components," Gençer says.

While considering all options, in the end the researchers found that pipelines were a less flexible option than trucks for transmission (although retrofitting gas pipelines could make hydrogen pipelines cost-effective for some uses), and trucking hydrogen gas was less expensive than trucking hydrogen in liquid form, since liquefaction has much higher energy consumption and capital costs than gas compression.

They then proposed a flexible scheduling and routing model for hydrogen trucks that would enable the vehicles to be used as both transmission and storage, as needed. Computationally, this was a particularly challenging step, according to He. "This is a very complex optimization model," he says. "We propose some techniques to reduce the complexity of the model."

The team chose to use judicious approximations for the number of trucks in the system and the needed commitment of SMR units, applying clustering and integer relaxation techniques. This enabled them to greatly improve the computational performance of their program without significantly impacting results in terms of cost and investment outcomes.

Case study of Northeast

Once the model was built, the researchers tested it by exploring the future hydrogen infrastructure needs of the U.S. Northeast under various carbon policy and hydrogen demand scenarios. Using 20 representative weeks from seven years of data, they simulated annual operations and determined the optimal mix of hydrogen infrastructure types given different carbon prices and the capital costs of electrolyzers.

"We showed that steam methane reforming of natural gas with carbon capture will constitute a significant fraction of hydrogen production and production capacity even under very high carbon price scenarios," Gençer says.

However, He says the results also suggest there is real synergy between the use of electrolysis for hydrogen generation and the use of compressed-gas trucks for transmission and storage. This finding is important, he explains, because "once we invest in these assets, we cannot easily switch to others."

He adds that trucks are a significantly more flexible investment than stationary infrastructure, such as pipes and transmission lines; trucks can easily be rerouted to serve new energy-generation facilities and new areas of demand, or even be left sitting to provide storage until more transmission capacity is needed. By comparison, building new electricity transmission lines or pipelines takes time—and they cannot be quickly adapted to changing needs.

"You have more renewables integrated into the system every day. People are installing rooftop solar panels, so you need more assets to transmit energy to other parts of the system," He says, explaining that a flexible supply chain can make the most of renewable generation. "A transmission line can take 10 years to build, during which time those renewables cannot be used as well. Using smaller-scale, distributed, portable storage or mobile storage can solve this problem in a timely manner."

Indeed, He and other colleagues recently conducted related research into the potential application of utility-scale portable energy storage in California. In a paper published in *Joule* in February, they showed that mobilizing energy storage can significantly increase revenues from storage in many regions and improve renewable energy integration. "It's more flexible" than such stationary solutions as additional grid capacity, He says. "When you don't need mobile storage anymore, you can convert it into stationary storage."

Now that He and his colleagues have created their hydrogen supply chain planning model, the next step, according to He, is to provide planners with broad access to the tool. "We are developing open-source code so people can use it to develop optimal assets for different sectors," He says. "We are trying to make the model better."

Kathryn M. O'Neill, MITEI correspondent

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G. He, D.S. Mallapragada, A. Bose, C.F. Heuberger, and E. Gencer. "Hydrogen supply chain planning with flexible transmission and storage scheduling." *IEEE Transactions on Sustainable Energy,* March 5, 2021. Online: doi.org/10.1109/TSTE.2021.3064015.

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Keeping humanity central to solving climate change

In MIT's School of Humanities, Arts, and Social Sciences, faculty, staff, and students generate research and ideas that help solve the economic, cultural, and political dimensions of the world's energy and climate challenges.

A solar engineer maintains the street lighting in her village of Tinginaput, India—a rural area not connected to the region's main electrical grid. Photo: Abbie Trayler-Smith/Panos Pictures/Climate Visuals

As a small child, Manduhai Buyandelger lived with her grandparents in a house unconnected to the heating grid on the outskirts of Ulaanbaatar, Mongolia. There, in the world's coldest capital city, temperatures can drop as low as minus 40 degrees Fahrenheit in the winter months.

"Once I moved further into the city with my parents, I had nightmares about my grandparents," recalls Buyandelger, now a professor of anthropology at MIT. "I felt so vulnerable for them. In the ger district where they lived, most people do not have central heating, and they warm their homes by making fire in their stoves. My grandparents didn't have heat. I was always worried about them getting up in their icy cold house, carrying buckets of coal from their shed back into the house, and then using a small shovel putting the coal in the stove. It has been more than 40 years since then, and life there is still very much like that."

With temperatures this harsh, having access to safe and affordable heat sources is critical for the citizens of Ulaanbaatar, especially for the 60% of the population living in the ger district. This suburban area of the city, known for its off-grid yurt-style dwellings, houses some of the city's most vulnerable citizens.

Traditionally, the households occupying the ger district kept their homes warm as Buyandelger's grandparents did, by using individual coal-burning stoves—contributing to Ulaanbaatar's other "claim to fame" as the world's most polluted capital city. In recent years, as air pollution reached levels twice as high as what the World Health Organization defined as "acutely hazardous," the Mongolian government took measures to combat this pollution. They banned the use of coal in ger district homes and enforced the use of cleaner-burning charcoal briquettes, which in turn created a new set of problems.

"A lot of people died," says Buyandelger. "The briquettes are toxic in a different way. Their instructions for burning are nuanced and require more oxygen in the house, which means people have to open their windows and doors, defeating their purpose." When burned incorrectly, these briquettes generate large amounts of carbon monoxide—an odorless, colorless, and toxic gas.

Establishing interdisciplinary collaborations

Enter Michael Short, the Class of '42 Associate Professor of Nuclear Science and Engineering (NSE) at MIT. He recognized the need for a safer, cleaner heat source and connected with Buyandelger, whose work in Mongolian anthropology was uniquely suited to aid these efforts. According to Buyandelger, "Oftentimes in history, people adjusted their behaviors so they can use technology. But we can do better and change the technology so that we don't necessarily jeopardize the people or culture."

With this goal in mind, Buyandelger, Short, and a team of students from NSE and anthropology have begun a collaboration to study the particularities of the local culture, environment, political climate, and economy in Ulaanbaatar to inform their work designing a sustainable, flameless thermal heat source made from molten nitrate salts. Once Covid-19 restrictions have lifted, they plan to travel to Mongolia where they will live in the ger district with those they aim to help, conducting ethnographic participant observations and extensive interviews to prototype a useful heat bank, observe its functionality in person, and make adaptations and improvements as needed.

For the students, the goal is two-fold: They will be trained in "anthropologically informed engineering" and see first-hand the benefits of developing a product with the end user in mind from the outset, and they will see how targeted, well-informed engineering can empower citizens and in turn preserve democracy.

"Our core hypothesis is that clean fuel independence from the government will foster democratization and prevent setbacks to authoritarianism," says Buyandelger. She explains that the people in the ger district are heavily dependent on the government: They must agree to use these dangerous fuels or else they will not qualify for other vital government subsidies and food programs. "We want to see if implementing the heat banks would help generate a more open and free society."

Understanding human complexities

When thinking about climate change and energy challenges across the globe, a lot of emphasis is put on what we can do with technology and policy to enact change. But, as illustrated in the Ulaanbaatar project, there is an important, undeniable element that is central: people.

"For scholars doing this research, if they don't include the political, social, and cultural dimensions, it is an incomplete project," says Melissa Nobles. She is the Kenan Sahin Dean of the MIT School of Humanities, Arts, and Social Sciences (MIT SHASS), as well as a professor of political science.

MIT SHASS is home to 13 academic fields, including anthropology, history, international studies, economics, and music and theater arts—all contributing to understanding the world's many human complexities. Part of the school's mission is to generate research and ideas that can change the world for the better, and it helps do this by informing public policy, educating leading science communicators, and shedding light on the cultural barriers that prevent people, organizations, and governments from supporting effective environmental policies and practices.

"Human motivation is hugely complicated," says Nobles. "The science has been clear on climate change, and it has been clear for a while; but as we see, the facts don't change people's behavior. You have to actually get people to ingest it intellectually and emotionally, because part of the resistance is rooted in fears of uncertainty: How am I going to have to change my life? What does it mean for my day-to-day? What does it mean for future generations?"

This question of the day-to-day was something that stuck out to Buyandelger when thinking about the cultural and social challenges their heat bank might face: "How do we distribute this? How heavy is it; will people be able to carry it? Who in the household will receive it? Can the temperature be altered for cooking?"

Integrating climate into curriculum

In MIT's SHASS classrooms, students learn to think critically about these big socio-political questions through some 30 courses that tackle climate and energy topics. Presented through rigorous humanities and social science lenses, the subjects range from history to literature to economics to political science to philosophy.

Courses include "The ethics of climate change," a moral philosophy class in which students explore the ethical implications of a rapidly warming world; "Reading climate through media," in which students learn how contemporary

A woman in Bangladesh cooks using biogas that her family makes from cow dung daily. In 2011, her family purchased a biogas plant for 350 U.S. dollars. They use the plant for personal consumption, including as a cleaner, cheaper cooking option. But not every household in their village can afford to buy one. Photo: Vidura Jang Bahadur/UN Women Asia and the Pacific/Climate Visuals media shapes public perceptions about climate issues, as well as how to craft effective climate stories and messages themselves; and "Environmental history," which explores the influence of planetary life and conditions on human history, and the reciprocal influence of people on the earth.

Clare Balboni, the 3M Career Development Assistant Professor of Environmental Economics, teaches graduate- and undergraduate-level courses on environmental policy and economics. The undergraduate-level course, which was taught in spring 2021 for the first time in several years, fulfills an elective requirement for MIT's Energy Studies Minor. Balboni joined the Department of Economics in 2019 and has since been working toward making environmental economics a core topic in the department.

"It's a really exciting time in environmental economics, and there is a tremendous amount of interest from the student body," Balboni says. "There is a long-standing tradition of theoretical work in this area, but more recently there has also been an upsurge in related empirical work. This reflects in part increased awareness and political and policy focus on environmental issues, but also enormous opportunities presented by new data sources, which make it possible to study environmental phenomena in ways that we weren't previously able to do."

She explains that economic studies can be key to informing effective climate solutions. "Understanding economic incentives and human behavior and responses is crucial. For instance, pollutants and climate damages can affect a wide range of human outcomes—such as mortality and health, labor productivity, education, conflict, and crime—which it is critical to understand and quantify when thinking about environmental policy design and implementation."

A woman waters a field in the Zambezi Valley of Mozambique, a region where climate change has affected hundreds of thousands of people largely dependent on rain-fed subsistence agriculture. An irrigation project run by Save the Children with UKaid support from the British government has helped improve their resilience to the many impacts of climate change such as drought and recurring floods. Photo: Marcos Villalta/Save the Children/Climate Visuals

A growing area of interest at MIT SHASS is how to continue incorporating climate into its curriculum across all of its varied academic disciplines. As climate change issues become an even more important topic in national legislation and policy making—especially with the new Biden-Harris administration in office—Nobles expects research and teaching to follow suit.

She explains that "what literature does, what music does, what art can do, what studying philosophy, culture, politics, and economics can do, is help students understand why it's so complicated for climate change efforts to move forward, and then, what they can do to help."

Kelley Travers, MITEI

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"Solving Climate: Humanistic Perspectives from MIT" is an ongoing series in which faculty, students, and alumni in the humanistic fields share perspectives that are significant for solving climate change and mitigating its myriad social and ecological impacts. To read the commentaries and stories, go to bit.ly/solving-climate.

Energy class dives into global problem of technology waste

While green energy solutions often rely on new technology, MIT students who took STS.032 Energy, Environment, and Society in fall 2020 discovered that even many promising innovations share a downside—electronics waste (e-waste).

Professor Clapperton Chakanetsa Mavhunga of the Program in Science, Technology, and Society teaches Energy, Environment, and Society, which in fall 2020 focused on the environmental and health consequences of improperly discarded electronics waste. Photo courtesy of Professor Mavhunga

"We've been using energy technologies that work well for our needs now, but we don't think about what happens 30 years in the future," says Jemma Schroder '24, a student in the class who learned that waste from solar panels, for example, is on the rise. The International Renewable Energy Agency has projected that, given the current rate of accumulation, the world will have amassed 78 million metric tons of such waste by 2050.

"We're trying to dig ourselves out of the pit, but we're just digging ourselves another pit," Schroder says. "If you're really aiming for sustainability, you have to think about all aspects of the problem."

Providing context for energy and sustainability issues is the major goal of STS.032, an elective for the Energy Studies Minor. "I understand the imperative that we need energy, we need electronic goods, but the environment is an afterthought. That's a big mistake," says Professor Clapperton Chakanetsa Mavhunga of the Program in Science, Technology, and Society, who teaches the class.

"We can no longer just focus on happy stories about technology," says Mavhunga, who serves on the Energy Minor Oversight Committee, a subcommittee of the Energy Education Task Force of the MIT Energy Initiative. "What I try to do is place energy in everyday life and to show issues everyday people are grappling with."

To that end, every year Mavhunga identifies a specific energy challenge and asks students in STS.032 to tackle it. "It's very much a problem-centered approach to the energy curriculum," he says.

Global perspective

During the fall 2020 term, Mavhunga's students spent eight weeks exploring the global landscape of energy and electronics waste, including cast-off cell phones and computers but also retired parts for solar panels. Topics covered ranged from the interplay of energy, race, inequality, poverty, and pollution in the United States to the dumping and innovative recycling of e-waste in Africa.

"We take a world tour, looking at how things are made, how they travel illegally around the world," Mavhunga says, noting that many cast-off electronics—and their associated pollutants—end up in the Global South. "There is this planned obsolescence at the level of design," he adds. "And the question of what to do with the waste has not been really discussed."

Students in STS.032 say they were shocked to learn that many solar panels are already becoming obsolete and that designers did not plan well for end-of-life reuse or recycling. "Solar panels only last 20 or 30 years, so what happens to them after they stop working is a problem," Schroder says. "Many can't be recycled, or they can be but it's too expensive to do so. So, people end up illegally shipping them off to sit in a waste dump."

"It never really occurred to me that electronics waste, especially solar waste, was such a big issue," says Julian Dubransky '21, who is majoring in humanities and engineering. "I'd argue it's one of the most important things I learned at MIT."

Waste hazards

STS.032 requires two individual papers and culminates in a final group research paper, which this term focused on characterizing the problems associated with solar and electronics waste and proposing solutions.

In their final paper, the students noted some of the hazards of electronics waste, including harmful chemicals such as lead, cadmium, and other known carcinogens, which can leach into the soil and contaminate water supplies. "In East African waste dumps, acids and chemicals from solar panels, lead-acid batteries, and lithium batteries are commonly drained directly into the ground to allow the metal components to be melted down and resold," the students wrote.

It's also common to burn the plastic off wires to recover valuable copper, even though the process generates toxic fumes, Schroder says. "It's not a priority for people to deal with these pollutants, though they are getting into land and water and deteriorating the health of everyone," she says, because the waste is being processed in areas where subsistence is the higher priority.

In their Energy, Environment, and Society class, students learned that their discarded cell phones and computers as well as retired parts of solar panels often end up in dumps like this one—the Richmond landfill in Bulawayo, the second largest city in Zimbabwe. Unless properly managed, such landfills can pose serious environmental and public health hazards. Photo: Charles Nyembe

The students conclude that addressing the problem of electronics waste will require more public awareness of the environmental and human health consequences of improperly discarded waste. "Tech waste is a big form of waste that we don't really talk about or see," Schroder says.

"You have to expose these problems and make people aware of them," Dubransky says, adding that the challenge of addressing electronics waste is more about the will than the way. "There isn't any true waste product if you can figure out how to reuse it or recycle it."

Innovative recycling

Underscoring that point, STS.032 provided students with several examples of innovative recycling efforts, ranging from simply using water bottles filled with dirt as building blocks to creating new electronics out of the old. "I don't know what I would do if someone gave me a pile of old electronics pieces, but they've created all these amazing machines, even 3D printers, from recycled tech," Schroder says, referring to entrepreneurs across the continent who have built businesses from electronics waste dumped in Africa (WoeLab in Togo is one example). "It's really inspiring."

Investigating what different communities do with waste is important, because it gives students the chance to see the problem from a new perspective, Mavhunga explains. "Different places in the world are connected, dealing with the same issues in different ways," he says. "Knowledge doesn't just come from universities and books. Knowledge can also come from people on the ground."

The students in STS.032 were able to identify some big-picture challenges to addressing electronics waste—notably the worldwide problem of inconsistent regulation—but they also had personal takeaways from the class.

Schroder, for example, says she won't be upgrading her phone anytime soon. That's because now that she understands the problem of electronics waste, she wants to do something about it.

"If you see a coal factory or a coal burner, you see the fumes rising up," she notes. "What you don't see is the phone you break and just throw out—you don't see what happens to that. The lack of awareness of what happens to these devices is a really big problem."

The students hope awareness will drive demand for solutions, such as products that are designed for reuse and recycling. "Lack of awareness is probably the biggest issue we have in regard to the e-waste problem. If we're aware it's a problem, solutions can start flowing in," Dubransky says.

Mavhunga says he hopes STS.032 can help MIT students drive such solutions. "Places like MIT should be where this is done precisely because this is where we've got the engineers," he says. "We need more people at the table who design from an ethical, environmental, and social perspective."

Kathryn M. O'Neill, MITEI correspondent

MISTI pilots conversations in energy

While fall typically sees MIT International Science and Technology Initiatives (MISTI) programs gearing up to facilitate international summer internship and research experiences for MIT students, this year's changing global circumstances presented challenges to making in-country internships happen—but they also offered new opportunities for students to engage with organizations and leaders overseas.

Combining MISTI's network of hosts, students' interests in energy, the broader energy community at MIT, and the ease of connecting internationally via remote platforms, the inaugural run of MISTI Career Conversations: *Energy* was born.

MISTI operates in more than 25 different countries, offering a number of programming options to the MIT community, including internships and research, faculty research, and teaching programs. Many of these provide the opportunity to collaborate with industry or research institutions on energy topics.

"Our aim was to give our students the same opportunities to build their networks and share ideas with industry leaders through a virtual platform, as they would have during a MISTI internship," says April Julich Perez, MISTI's executive director. "While the Covid-19 pandemic has put a damper on international travel, programs such as MISTI Career Conversations have made it possible to bring our students and global partners together in exciting new ways."

The initial series of conversations focused on Denmark and India, two countries making critical strides in the movement toward green energy, but with their own methods and targets. Future series will expand to other topics and regions.

The MISTI Career Conversations: *Energy* program serves as an innovative pivot from international internships to a virtual seminar series. Images courtesy of MISTI Career Conversations

As an emerging economy with a rapidly growing population, India has set a target of 175 gigawatts of renewable energy capacity by 2022. The current areas of focus are wind and solar energy, with a strong emphasis on building out the transmission infrastructure. Indian organizations represented in this series included Sterlite Power, Shell Research Technology Center, Tata Power, and ReNew Power.

While it faces different challenges from India, Denmark has set ambitious goals for itself to offset the progression of climate change. By 2050, Denmark aims to be fossil fuel–free, and already around half of Denmark's energy needs are being met by renewable energy, most of that from wind power. Three companies represented Denmark during the first MISTI Career Conversations: *Energy* series: Ramboll, the international engineering consultancy with a focus on the green transition; Ørsted, a global leader in wind power and the largest energy company in Denmark; and GreenLab, a green industrial park and power-to-x facility.

Each company shared its unique and innovative approaches to the energy sector and the transition to renewable energy, both within the context of its country and the world. This allowed participants to ask questions related to their academic interests and future career goals.

"As an alum, it was rewarding to connect with current students and reconnect with the latest updates from campus," says Manya Rajan SM '10, chief asset officer at Sterlite Power. "I felt very comforted by the fact that the energy ecosystem is as thriving and dynamic as it can be in the context of today's situation. I look forward to staying in touch with the students through MISTI's various platforms and learning about the amazing work they are doing, and will do."

A cohort of dedicated students, including undergrad and graduate students from a variety of disciplines, was formed. All shared an interest in energy and the desire to network with professionals while discussing real-world issues.

"I was very keen on learning about the different energy solutions being deployed in different parts of the world, and the type of expertise, thinking, and experience it takes to make an impact in the field," says Awele Uwagwu, a senior pursuing an SB in chemical engineering and minor in energy studies. "Throughout the series, I did get this insight. It was clear to see that a country like India has significantly different challenges than a country like Denmark. I also learned about the different types of energy solutions deployed based on context, and I'm getting a better picture of where I want to fit into this."

Titan Hartono, a PhD student in mechanical engineering, reflected on being able to connect her research on photovoltaics to the "bigger picture" of

Manya Ranjan SM '10 of Sterlite Power (center) meets with the MISTI Career Conversations: *Energy* cohort. Ranjan noted that the opportunity to connect with current students confirmed for him that MIT's energy ecosystem continues to be thriving and dynamic.

energy challenges we are facing globally. "Working in a lab and conducting experiments created this sense of disconnection with what is actually going on in the electricity power market," she explains. "Getting connected with different companies in India and Denmark was exactly the opportunity I was looking for."

"I've always loved engaging with fellow MIT students about topics of energy and sustainability as a materials science major and energy studies minor, and I'm very glad I was able to do so as part of the MISTI Career Conversations series," says Anthony Cheng '20, who interned with GreenLab through MIT-Denmark and later joined their team in Skive, Denmark. "Through MISTI's excellent connections and support, I've been working at the Danish green industrial park startup GreenLab for the past few months, and it was exciting to be able to help share GreenLab's vision for making an impact on industrial energy transitions and development."

Anurit Kanti, deputy manager–sustainability at ReNew Power, notes the value of industry-academia collaboration: "Engaging with MIT students from diverse backgrounds on various aspects of the energy transition, including digitization of the energy sector, was extremely fruitful. The discussion with the students was stimulating, and it makes us hopeful for top talent to be involved in this sector, which in turn will catalyze the energy transition."

Providing students an opportunity to connect their focus of study to real-life approaches in the energy sector and the energy transition conversation embodies the MIT spirit of "mens et manus" ("mind and hand"). Antje Danielson, director of education at the MIT Energy Initiative (MITEI), notes, "It is important for the outlook of our students to showcase companies that have clear strategies to achieve set climate goals. Our students want to know that they will have opportunities to contribute to a meaningful, visionary effort like the energy transition once they graduate."

Moving forward, MISTI and MITEI will continue to provide students with an opportunity to engage with leaders in the energy sector through robust programming and field trips that capitalize on the pressing issues both in the United States and around the world.

Christina Davies, MIT International Science and Technology Initiatives

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A second iteration in this series will run as a credit-bearing course in fall 2021, under the new title "MISTI Career Connections: *Energy*."

Awele Uwagwu: From gas to solar, bringing meaningful change to Nigeria's energy systems

Growing up, Awele Uwagwu's view of energy was deeply influenced by the oil and gas industry. He was born and raised in Port Harcourt, a city on the southern coast of Nigeria, and his hometown shaped his initial interest in understanding the role of energy in our lives.

"I basically grew up in a city colored by oil and gas," says Uwagwu. "Many of the jobs in that area are in the oil sector, and I saw a lot of large companies coming in and creating new buildings and infrastructure. That very much tailored my interest in the energy sector. I kept thinking: What is all of this stuff going on, and what are all these big machines that I see every day? The more sinister side of it was: Why is the water bad? Why is the air bad? And, what can I do about it?"

MIT senior Awele Uwagwu has co-founded a startup that aims to accelerate the adoption of solar energy in Nigeria, where widely used petrol-powered generators now emit pollutants that harm health and contribute to climate change. Photo: Mira Whiting Photography

Uwagwu has shaped much of his educational and professional journey around answering that question: "What can I do about it?" He is now a senior at MIT, majoring in chemical engineering with a minor in energy studies.

After attending high school in Nigeria's capital city, Abuja, Uwagwu decided to pursue a degree in chemical engineering and briefly attended the University of Illinois Urbana-Champaign in 2016. Unfortunately, the impacts of a global crash in oil prices made the situation difficult back in Nigeria, so he returned home and found employment at an oil services company working on a water purification process.

It was during this time that he decided to apply to MIT. "I wanted to go to a really great place," he says, "and I wanted to take my chances." After only a few months of working at his new job, he was accepted to MIT.

"At this point in my life I had a much clearer picture of what I wanted to do. I knew I wanted to be in the energy sector and make some sort of impact. But I didn't quite know how I was going to do that," he says.

With this in mind, Uwagwu met with Rachel Shulman, the undergraduate academic coordinator at the MIT Energy Initiative, to learn about the different ways that MIT is engaged in energy. He eventually decided to become an Energy Studies Minor and concentrate in energy engineering studies through the 10-ENG: Energy program in the Department of Chemical Engineering. Additionally, he participated in the Undergraduate Research Opportunities Program (UROP) in the lab of William H. Green, the Hoyt C. Hottel Professor in Chemical Engineering, focusing on understanding the different reaction pathways for the production of soot from the combustion of carbon.

After this engaging experience, he reconnected with Shulman to get involved with another UROP, this time with a strong focus in renewable energy. She pointed him toward Ian Mathews—a postdoc in the MIT Photovoltaic Research Laboratory and founder of Sensai Analytics—to discuss ways he could make a beneficial impact on the energy industry in Nigeria. This conversation led to a second UROP, under the supervision of Mathews. In that project, Uwagwu worked to figure out how cost-effective solar energy would be in Nigeria compared to petrol-powered generators, which are commonly used to supplement the unreliable national grid.

"The idea we had is that these generators are really, really bad for the environment, whereas solar is cheap and better for the environment," Uwagwu says. "But we needed to know if solar is actually affordable." After setting up a software model and connecting with Leke Oyefeso, a friend back home, to get data on generators, they concluded that solar was cost-comparable and often cheaper than the generators.

Powering up: The creation of a virtual solar energy marketplace for Nigeria

Armed with this information and another completed UROP, Uwagwu thought, "What happens next?" Quickly an idea started forming, so he and Oyefeso went to Venture Mentoring Services at MIT to figure out how to leverage this knowledge to start a company that could deliver a unique and much-needed product to the Nigerian market.

They ran through many different potential business plans and ideas, eventually deciding on creating software to design solar systems that are tailored to Nigeria's specific needs and context. Having come up with the initial idea, they "chatted with people on the solar scene back home to see if this is even useful or if they even need this."

Through these discussions and market research, it became increasingly clear to them what sort of novel and pivotal product they could offer to help accelerate Nigeria's burgeoning solar sector, and their initial idea took on a new shape: solar design software coupled with an online marketplace that connects solar providers to funding sources and energy consumers. In recognition of his unique venture, Uwagwu received a prestigious Legatum Fellowship, a program that offers entrepreneurial MIT students strong mentoring and networking opportunities, educational experiences, and substantial financial support.

Since its founding in the summer of 2020, their startup, Idagba, has been hard at work getting its product ready for market. Starting a company in the midst of Covid-19 has created a set of unique challenges for Uwagwu and his team, especially as they operate on a whole other continent from their target market.

"We wanted to travel to Lagos last summer but were unable to do so," he says. "We can't make the software without talking to the people and businesses who are going to use it, so there are a lot of Zoom and phone calls going on."

In spite of these challenges, Idagba is well on its path to commercialization. "Currently we are developing our minimum viable product," comments Uwagwu. "The software is going to be very affordable, so there's very little barrier for entry. We really want to help create this market for solar."

In some ways, Idagba is drawing lessons from the success of Mo Ibrahim and his mobile phone company, Celtel. In the late '90s, Celtel was able to quickly and drastically lower the overall price of cell phones across many countries in Africa, allowing for the widespread adoption of mobile communication at a much faster pace than had been anticipated. To Uwagwu, this same idea can be replicated for solar markets. "We want to reduce the financial and technical barriers to entry for solar like he did for telecom."

This won't be easy, but Uwagwu is up to the task. He sees his company taking off in three phases. The first is getting the design software online. After that has been accomplished—by mid-2021—comes the hard part: getting customers and solar businesses connected and using the program. Once they have an existing user base and proven cash flow, the ultimate goal of the company is to create and facilitate an ecosystem of people wanting to push solar energy forward. This will make Idagba, as Uwagwu puts it, "the hub of solar energy in Nigeria." Idagba has a long way to go before reaching that point, but Uwagwu is confident that the building blocks are in place to ensure its success.

After graduating in June, Uwagwu will be taking up a full-time position at the prestigious consulting firm Bain and Company, where he plans to gain even more experience and connections to help grow his company. This opportunity will provide him with the knowledge and expertise to come back to Idagba and, as he says, "commit my life to this."

"This idea may seem ambitious and slightly nonsensical right now," says Uwagwu, "but this venture has the potential to significantly push Nigeria away from unsustainable fossil fuel consumption to a much cleaner path."

Turner Jackson, MITEI

David Fischer: Pushing the envelope with fusion magnets

"At the age of between 12 and 15, I was drawing; I was making plans of fusion devices."

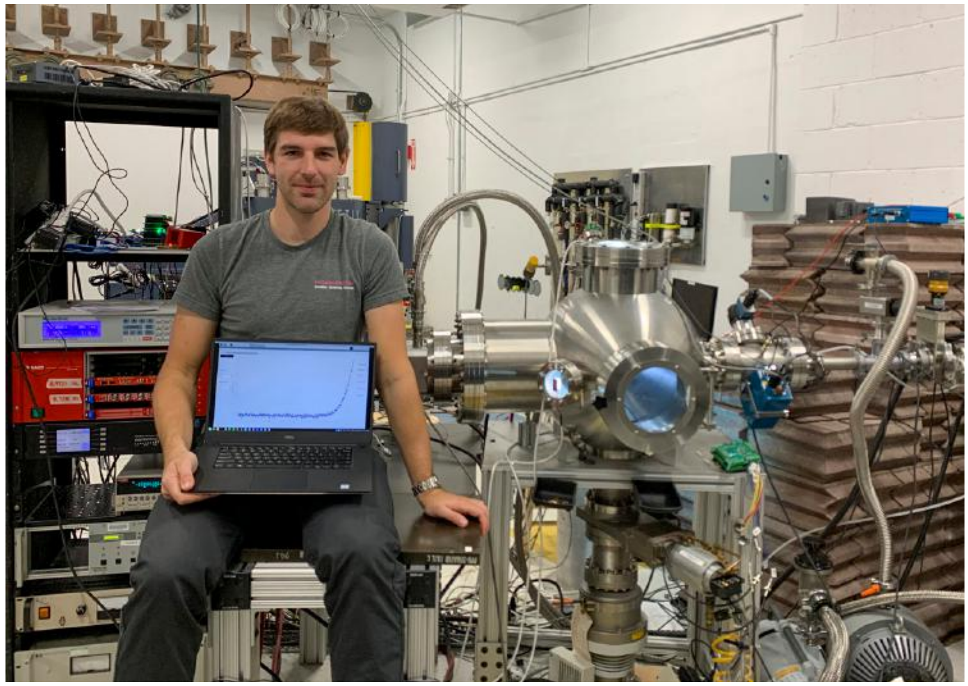
David Fischer remembers growing up in Vienna, Austria, imagining how best to cool the furnace used to contain the hot soup of ions known as plasma in a fusion device called a tokamak. With plasma hotter than the core of the sun being generated in a donut-shaped vacuum chamber just a meter away from these magnets, what temperature ranges might be possible with different coolants, he wondered.

"I was drawing these plans and showing them to my father," he recalls. "Then somehow I forgot about this fusion idea."

Now starting his second year at the Plasma Science and Fusion Center (PSFC) as a postdoctoral associate and a new Eni-sponsored MIT Energy Fellow through the MIT Energy Initiative, Fischer has clearly reconnected with the "fusion idea." And his research revolves around the concepts that so engaged him as a youth.

Fischer's early designs explored a popular approach to generating carbon-free, sustainable fusion energy known as "magnetic confinement." Since plasma responds to magnetic fields, the tokamak is designed with magnets to keep the fusing atoms inside the vessel and away from the metal walls, where they would cause damage. The more effective the magnetic confinement, the more stable the plasma can become, and the longer it can be sustained within the device.

Fischer is working on ARC, a fusion pilot plant concept that employs thin high-temperature superconductor (HTS) tapes in the fusion magnets. HTS allows much higher magnetic fields than would be possible from conventional superconductors, enabling a more compact tokamak design. HTS also allows the fusion magnets to operate at higher temperatures, greatly reducing the required cooling.



David Fischer sits beside the experiment's vacuum chamber (illuminated in blue), where the high-temperature superconductor tapes will be mounted for proton irradiation and *in situ* transport current measurement. His laptop shows data obtained in such measurements—the basis for determining the critical current. Photo: Zoe Fisher

Fischer is particularly interested in how to keep the HTS tapes from degrading. Fusion reactions create neutrons, which can damage many parts of a fusion device, with the strongest effect on components closest to the plasma. Although the superconducting tapes may be as much as a meter away from the first wall of the tokamak, neutrons can still reach them. Even in reduced numbers and after losing most of their energy, the neutrons damage the microstructure of the HTS tape and over time change the properties of the superconducting magnets.

Much of Fischer's focus is devoted to the effect of irradiation damage on the critical currents, the maximum electrical current that can pass through a superconductor without dissipating energy. If irradiation causes the critical currents to degrade too much, the fusion magnets can no longer produce the high magnetic fields necessary to confine and compress the plasma.

Fischer notes that it is possible to significantly reduce damage to the magnets by adding more shielding between the magnets and the fusion plasma. However, this would require more space, which comes at a premium in a compact fusion power plant.

"You can't just put infinite shielding in between. You have to learn first how much damage can this superconductor tolerate, and then determine how long do you want the fusion magnets to last. And then design around these parameters."

Fischer's expertise with HTS tapes stems from studies at Technische Universität Wien (Vienna University of Technology), Austria. Working on his master's degree in the low temperature physics group he was told that a PhD position was available researching radiation damage on coated conductors, materials that could be used for fusion magnets.

Recalling the drawings he shared with his father he thought, "Oh, that's interesting. I was attracted to fusion more than ten years ago. Yeah, let's do that."

The resulting research on the effects of neutron irradiation on high-temperature superconductors for fusion magnets, presented at a workshop in Japan, got the attention of PSFC nuclear science and engineering professor Zach Hartwig PhD '14 and Commonwealth Fusion Systems Chief Science Officer Brandon Sorbom PhD '17.

"They lured me in," he laughs.

Like Fischer, Sorbom had explored in his own dissertation the effect of radiation damage on the critical current of HTS tapes. What neither researcher had the opportunity to examine was how the tapes behave when irradiated at 20 kelvins (K), the temperature at which the HTS fusion magnets will operate.

Fischer now finds himself overseeing a proton irradiation laboratory for PSFC director Dennis G. Whyte. He is building a device that will not only allow him to irradiate the superconductors at 20 K, but also immediately measure changes in the critical currents.

He is glad to be back in the NW13 lab, fondly known as "The Vault," working safely with graduate and Undergraduate Research Opportunities Program student assistants. During his Covid-19 lockdown he was able to work from home on programming a measurement software, but he missed the daily connection with his peers.

"The atmosphere is very inspiring," he says, noting some of the questions his work has recently stimulated. "What is the effect of the irradiation temperature? What are the mechanisms for the degradation of the critical currents? Could we design HTS tapes that are more radiation resistant? Is there a way to heal radiation damage?"

Fischer may have the chance to explore some of his questions as he prepares to coordinate the planning and design of a new neutron irradiation facility at MIT.

"It's a great opportunity for me," he says. "It's great to be responsible for a project now, and see that people trust that you can make it work."

Paul Rivenberg, MIT Plasma Science and Fusion Center

Via Separations: MITEI spin-off takes aim at industrial decarbonization

If you wanted to get pasta out of a pot of water, would you boil off the water, or use a strainer? While home cooks would choose the strainer, many industries continue to use energy-intensive thermal methods of separating out liquids.

In some cases, that's because it's difficult to make a filtration system for chemical separation, which requires pores small enough to separate atoms. In other cases, membranes exist to separate liquids, but they are made of fragile polymers, which can break down or gum up in industrial use.

Via Separations, a startup that emerged from MIT in 2017, has set out to address these challenges with a membrane that is cost-effective and robust. Made of graphene oxide (a "cousin" of pencil lead), the membrane can reduce the amount of energy used in industrial separations by 90%, according to Shreya Dave PhD '16, company co-founder and CEO.

This is valuable because separation processes account for about 22% of all in-plant energy use in the United States, according to Oak Ridge National Laboratory. By making such processes significantly more efficient, Via Separations plans both to save energy and to address the significant emissions produced by thermal processes. "Our goal is eliminating 500 megatons of carbon dioxide emissions by 2050," Dave says.

Shreya Dave PhD '16 (center) co-founded Via Separations with Professor Jeffrey Grossman (left) and Brent Keller PhD '16. Photo: Shun Liang, courtesy of Via Separations

Via Separations is piloting its technology this spring at a U.S. paper company and expects to deploy a full commercial system there in the spring of 2022. "Our vision is to help manufacturers slow carbon dioxide emissions next year," Dave says.

MITEI Seed Grant

The story of Via Separations begins in 2012, when the MIT Energy Initiative (MITEI) awarded a Seed Fund grant to Professor Jeffrey Grossman, who is now the Morton and Claire Goulder and Family Professor in Environmental Systems and head of MIT's Department of Materials Science and Engineering; Grossman was pursuing research into nanoporous membranes for water desalination. "We thought we could bring down the cost of desalination and improve access to clean water," says Dave, who worked on the project as a graduate student in Grossman's lab.

There she teamed up with Brent Keller PhD '16, another Grossman graduate student and a 2016-2017 ExxonMobil-MIT Energy Fellow, who was developing lab experiments to fabricate and test new materials. "We were early comrades in figuring out how to debug experiments or fix equipment," says Keller, Via Separations' co-founder and chief technology officer. "We were fast friends who spent a lot of time talking about science over burritos."

Dave went on to write her doctoral thesis on using graphene oxide for water desalination, but that turned out to be the wrong application of the technology from a business perspective, she says. "The cost of desalination doesn't lie in the membrane materials," she explains.

So, after Dave and Keller graduated from MIT in 2016, they spent a lot of time talking to customers to learn more about the needs and opportunities for their new separation technology. This research led them to target the paper industry, because the environmental benefits of improving paper processing are enormous, Dave says. "The paper industry is particularly exciting because separation processes just in that industry account for more than 2% of U.S. energy consumption," she says. "It's a very concentrated, high-energy-use industry."

Most paper today is made by breaking down the chemical bonds in wood to create wood pulp, the primary ingredient of paper. This process generates a byproduct called black liquor, a toxic solution that was once simply dumped into waterways. To clean up this process, paper mills turned to boiling off the water from black liquor and recovering both water and chemicals for reuse in the pulping process. (Today, the most valuable way to use the liquor is as biomass feedstock to generate energy.) Via Separations plans to accomplish this same separation work by filtering black liquor through its graphene oxide membrane.

"The advantage of graphene oxide is that it's very robust," Dave says. "It's got carbon double bonds that hold together in a lot of environments, including at different pH levels and temperatures that are typically unfriendly to materials."

Such properties should also make the company's membranes attractive to other industries that use membrane separation, Keller says, because today's polymer membranes have drawbacks. "For most of the things we make—from plastics to paper and gasoline—those polymers will swell or react or degrade," he says.

Graphene oxide is significantly more durable, and Via Separations can customize the pores in the material to suit each industry's application. "That's our secret sauce," Dave says, "modulating pore size while retaining robustness to operate in challenging environments."

"We're building a catalog of products to serve different applications," Keller says, noting that the next target market could be the food and beverage industry. "In that industry, instead of separating different corrosive paper chemicals from water, we're trying to separate particular sugars and food ingredients from other things."

Future target customers include pharmaceutical companies, oil refineries, and semiconductor manufacturers, or even carbon capture businesses.

Scaling up

Dave, Keller, and Grossman launched Via Separations in 2017—with a lot of help from MIT. The company's first capital investment came from The Engine, a venture firm founded by MIT to support "tough tech" companies (tech businesses with transformative potential but long and challenging paths to success). The founders also received advice and support from MIT's Deshpande Center for Technological Innovation, Venture Mentoring Service, and Technology Licensing Office. In addition, Grossman continues to serve the company as chief scientist.

"We were incredibly fortunate to be starting a company in the MIT entrepreneurial ecosystem," Keller says, noting that The Engine support alone "probably shaved years off our progress."

Already, Via Separations has grown to employ 17 people, while significantly scaling up its product. "Our customers are producing thousands of gallons per minute," Keller explains. "To process that much liquid, we need huge areas of membrane."

Via Separations' manufacturing process, which is now capable of making more than 10,000 square feet of membrane in one production run, is a key competitive advantage, Dave says. The company rolls 300-400 square feet of membrane into a module, and modules can be combined as needed to increase filtration capacity.

The goal, Dave says, is to contribute to a more sustainable world by making an environmentally beneficial product that makes good business sense. "What we do is make manufacturing things more energy-efficient," she says. "We allow a paper mill or chemical facility to make more product using less energy and with lower costs. So, there is a bottom-line benefit that's significant on an industrial scale."

Keller says he shares Dave's goal of building a more sustainable future. "Climate change and energy are central challenges of our time," he says. "Working on something that has a chance to make a meaningful impact on something so important to everyone is really fulfilling."

Kathryn M. O'Neill, MITEI correspondent

To hear more from Shreya Dave PhD '16 about starting Via Separations, listen to MITEI podcast #27, "Climate tech startups" (energy.mit.edu/podcast/climate-tech-startups).

Collaborators in climate action: Symposium highlights ambitious goals of MIT–industry research

MIT is committed to driving the transition to a low-carbon world, throwing the full weight of its research forces into transformative technologies for reducing greenhouse gas emissions. But "MIT can't solve climate change alone," said Maria T. Zuber, MIT's vice president for research and E.A. Griswold Professor of Geophysics, speaking at a virtual symposium on March 18, 2021.

When MIT initiated its first Climate Action Plan in 2015, a key tenet, said Zuber, was "engagement with actors and entities outside of MIT." As the Institute prepares to issue an updated version of the plan later this spring, this engagement forum, "Research collaborations to decarbonize the energy system," was conceived as an opportunity for the MIT community to learn about and comment on some of the low-carbon research projects between MIT and key outside collaborators. It was co-hosted by the Office of the Vice President for Research and the MIT Energy Initiative (MITEI).

"With vignettes of current or recent engagement activities, we seek to share a small handful of examples of how working with industry has catalyzed progress in the electric power sector, life-cycle analysis to inform decarbonization efforts, and fusion energy, to name a few," said MITEI Director Robert C. Armstrong, the Chevron Professor of Chemical Engineering, in his introductory remarks.

Symposium speakers, who included MIT faculty and scientists, industry liaisons, and venture capital leaders, made clear that joining forces yields concrete benefits—not simply in specific technologies or sectors, but in the kind of large-scale, market-based solutions required to meet the climate crisis.

Wind, electric vehicles, and nuclear

Take, for instance, the case of Iberdrola, a Spanish-based multinational electric utility with a large renewables portfolio, which is launching a vast fleet of offshore wind farms around the world. As a senior asset performance analysis engineer for the company, Sofia Koukoura found help in modeling the operation of these turbines from Kalyan Veeramachaneni, a principal research scientist with the MIT Laboratory for Information and Decision Systems.

Veeramachaneni harnessed machine learning to predict component failures and likely repairs affecting the longevity of these turbines, providing Koukoura with "flexible, reproducible, and scalable solutions," she said. "Bridging the gap between development and deployment of a project is a big leap, and the team at MIT is helping us do that."

Other panels in this session, moderated by Angela Belcher, the James Mason Crafts Professor of Biological Engineering and Materials Science and Engineering, and head of the Department of Biological Engineering, demonstrated the reciprocal nature of MIT's research with industry associates.

One such case: MITEI research scientist Emre Gençer has developed a life-cycle assessment tool called SESAME (Sustainable Energy Systems Analysis Modeling Environment) to enable a systems-level understanding of the environmental impact and fuel emissions reduction potential of a spectrum of interrelated energy technologies.

ExxonMobil's Research and Engineering Company—a sponsor of MITEI's Mobility of the Future study—engaged with Gençer to use SESAME for modeling the emissions impacts of switching from internal combustion engine vehicles to hybrid, battery electric, and hydrogen fuel cell vehicles in different regions of the United States. Jennifer Morris, a research scientist with both MITEI and the MIT Joint Program on the Science and Policy of Global Change, provided the various policy scenario projections for the Mobility of the Future study.

The resulting studies proved useful not just to ExxonMobil, but to the MIT scientists as well.

"In academia, we can come up with solutions, but if they're not implementable, they're not as valuable, especially during a climate crisis," said Gençer. "These connections with industrial sponsors are valuable, because they provide reality checks on our technological and economic assumptions," said Morris. "These are real-world challenges that make our applications relevant and have real-world impact." The goal is to make these tools widely available to policy makers, industry, and other stakeholders to inform decision making that can drive decarbonization.

An example from another research domain: Michael Short '05, SM '10, PhD '10, Class of '42 Associate Professor of Nuclear Science and Engineering (NSE), had been searching for a solution to a vexing, decades-old issue for light water nuclear reactors—the deposition of corrosive deposits on nuclear fuel, which can lead to reactor downtime.

When Short's lab cracked this problem of fuel rod fouling, a major U.S. clean energy provider recognized that it might be valuable for reducing costs on its nuclear fleet. With support from this company, Short's lab is now busy developing materials with better resistance to these deposits, which could help keep existing reactors producing clean energy for decades to come.

Beyond such technological advances, Short notes there are less tangible yet significant rewards to the joint enterprise with industry. When "students have frequent, primary contact with an industry sponsor, they learn they are not just first authors on papers but on patents as well, giving them a sense of what problems they want to work on and what to do with their lives," he said. If students solve a problem in science, they will see "someone is ready to snap it up and make an impact on the carbon issue."

Solar and fusion breakthroughs

In recent years, alliances formed between MIT researchers and outside companies have not merely sparked novel carbon-cutting technologies, but laid the groundwork for pathbreaking spinoffs, and even potential new industries. Two panels moderated by Anne White, NSE department head and MIT School of Engineering Distinguished Professor of Engineering, featured instructive cases.

When Italian energy company Eni first paired up with MIT in 2008, founding the Solar Frontiers Center (SFC), the initial goal was to "explore everything beyond silicon," said Massimiliano Pieri, Eni's cleantech director at Eni Next, Eni's corporate venture capital organization. After dozens of SFC projects, which have involved a small army of graduate students, generated many patent filings and produced hundreds of research papers, it is readily apparent that MIT "has dramatically benefited," said Vladimir Bulović, a professor of electrical engineering and the Fariborz Maseeh Chair in Emerging Technology. Among the results of this mutual venture: a new class of super-thin, flexible, and lightweight materials that could vastly expand the use of solar energy.

The first webinar in a two-part series aimed at giving members of the MIT community the opportunity to learn about and offer their thoughts on the benefits and challenges of working in collaboration with other organizations was held March 18, 2021. Image: Kelley Travers, MITEI

This long-lived collaboration has also served as the launchpad for such startups as Swift Solar, co-founded by Joel Jean SM '13, PhD '17, and Ubiquitous Energy, co-founded by Miles Barr SM '08, PhD '12, both of whom earned a *Forbes* 30 under 30 in Energy for innovations in the solar industry. Work with Eni at SFC "inspired me to start a career commercializing new solar technology," said Barr.

In 2016, when researchers in MIT's Plasma Science and Fusion Center (PSFC) saw a path to making commercial fusion energy a reality, they went big, searching for collaborators who could help "launch a new energy industry," said Dennis G. Whyte, PSFC director and Hitachi America Professor of Engineering. "It was high risk, but the idea resonated with us," said Pieri, whose Eni Next firm invested in the MIT spinoff, Commonwealth Fusion Systems (CFS).

With additional investment from Bill Gates' Breakthrough Energy Ventures and other leading investors in breakthrough energy technologies, said CFS CEO Bob Mumgaard SM '15, PhD '15, "We were able to attract talent from all sorts of disciplines much earlier than normally possible, start the company, and scale up quickly." CFS is now on a fast track to build the world's first net energy fusion machine, and from there, the first commercially viable fusion power plant, opening a window to limitless clean energy.

By symposium's end, participants had reached consensus: To achieve the urgent goals of the climate fight, whether by catalyzing new energy industries or deploying cost-effective, carbon-reducing applications, industry and academia must work cooperatively. "We truly need to step up our game—we simply don't yet have all the technologies we need to decarbonize our energy systems and our economy," said Zuber. "You've heard the phrase, 'Go big, or go home.' When it comes to climate change, going big is imperative, because Earth is our home."

On April 1, 2021, the Office of the Vice President for Research co-hosted another forum, "Viewpoints from the MIT community engaging on climate change: An all-of-MIT approach," this one in conjunction with the Environmental Solutions Initiative.

Leda Zimmerman, MITEI correspondent

To watch a video of the first forum in this two-part series, please go to www.youtube.com/watch?v=cDEDz3FKzwY.

3 Questions: Ernest Moniz on the future of climate and energy under the Biden-Harris administration

Climate and energy are two key areas on the Biden-Harris administration's agenda. Here, Robert C. Armstrong, director of the MIT Energy Initiative (MITEI), asks Ernest J. Moniz—professor emeritus post-tenure, MITEI's founding director, special advisor to MIT President L. Rafael Reif, and former U.S. Secretary of Energy—about key challenges and targets that the new administration should consider to accelerate significant progress in these areas.

Q What are your initial thoughts on what the top priority items should be for the Biden-Harris administration?

A First of all, I think we should start off by saying that it's pretty clear that the president is going to move out smartly on energy and climate. His appointments speak volumes, starting out with John Kerry in this new international envoy position; with Gina McCarthy; Brian Deese in the White House; Jennifer Granholm as the secretary of energy, who, as the governor of Michigan, did a lot with renewables and transportation; and the choice of Janet Yellen in the treasury with her well-known commitment to carbon emissions pricing.

It's pretty convincing that the Biden-Harris administration is in fact going to carry through with its "whole of government" approach to addressing climate. Now, in terms of priorities going forward, I think it's important to distinguish between the types of actions that he can take. Clearly, there will be a large package of executive actions that can be taken without Congress.

Frankly, some of those will be reversing what Trump rolled back. Some examples of rollback to Obama-Biden rules, possibly further strengthened under Biden-Harris, could include Corporate Average Fuel Economy (CAFE) standards for auto efficiency and methane emissions rules.

There will also be a restart of some major Obama-Biden activities. One that I was very close to while energy secretary was energy efficiency standards. During the Obama period, the Department of Energy issued more than 50 energy-efficiency standards. We're talking more than half a trillion dollars of consumer savings and about two to three gigatons of CO_2 avoided cumulatively to 2030. You're going to see that come out like gangbusters, maybe even more aggressive than when we were in the Obama administration.

Rejoining the Paris Agreement is a no-brainer. Getting in as a notification on Day One, and then 30 days later we're in. Now, what do you do with it? The very early announcement of John Kerry's position as international climate envoy was a clear statement that we don't want to just rejoin Paris, we want to reestablish a leadership position. Other countries haven't taken a four-year vacation on this. They've been working hard at it. We have to earn our place back at the table. A major test in the next few months will be formulation of a much more aggressive nationally determined contribution for 2030 than that adopted for 2025 at the Paris climate meeting just over five years ago, while also describing a domestic program that can credibly reach the goal. It will be tough to thread this needle.

These are only a few highlights of things that will be reestablished, but there will also be some new elements as well. For example, I believe that he will order all the financial regulatory agencies to put corporate climate risk disclosures very high on the agenda, reinforcing what the private banks and investors do in terms of the environmental, social, and corporate governance movement. It's going to be a major executive package that the administration can put in place.

Q There have been a lot of interesting climate and energy experiments and aggressive programs at the state and regional levels around the country. What lessons can be learned from these examples, and how can we take national legislative action that leverages what we have already learned?

A Despite the newfound Democratic majority in the Senate, I don't think we should be fooled into thinking that it's going to be easy to get comprehensive legislation immediately. Frankly, there's a lot of work to do in bringing the Democrats together in terms of what kinds of programs are actually needed. If we assume, and I do assume, that once again we will not have comprehensive legislation on matters such as significant carbon emissions pricing anytime soon, state and city leadership will continue to be very important because in these past few years, clearly states and cities have been the ones leading the charge, often with opposition of the federal government.

Moving forward, there will be synergy between what the states and cities and the administration want to do. One should not underestimate how that will free up a lot of state and city initiatives on the path to the U.N. Climate Conference in Glasgow in late 2021, reinforcing a magic year of repositioning America on climate and clean energy. For example, I'm expecting that the considerable number of net-zero declarations by cities and states (and companies, too) will only be strengthened. Clearly, national

Ernest Moniz, professor emeritus post-tenure, special advisor to the MIT president, and founding director of the MIT Energy Initiative, answers three questions about what to expect from the Biden-Harris administration. Photo: Bryce Vickmark

comprehensive legislation is desired and will eventually be very important, but we've always emphasized that, even with national legislation, we should never lose sight of the fact that low-carbon solutions are fundamentally regional in nature. This is a key direction that the Biden-Harris administration can go in even without comprehensive legislation. Facilitating and encouraging these kinds of regionally focused solutions is the only way we're going to reach the net-zero objective.

Going back to Congress, there are two areas that I feel are ripe for congressional bipartisan action: innovation and infrastructure. Innovation is where the Congress in the last four years has shown promising bipartisan support. This is the decade where we need supercharged innovation because if we don't get that addressed in this decade, we're not going to have the scale potential in the 2030s and '40s that we're going to need for the mid-century net-zero goal.

Congress knows that they cannot kick the can down the road any further on infrastructure. The money has to be found and that will include as an important subset, energy infrastructure. That will obviously include the electricity system, for example, but it will also include things such as the infrastructure that is needed for large-scale carbon management and the infrastructure for large-scale, multisectoral hydrogen development. With innovation and infrastructure, I do believe that we'll be able to garner strong bipartisan support. Clearly once we get into more difficult areas, that may take more time.

Q Many argue that clean power generation alone will not be enough to address the climate and energy crisis and that carbon removal technologies will prove to be essential to get us there. This begs the question about what the Biden-Harris administration might do to address these areas. How could they incentivize carbon capture, utilization, and sequestration (CCUS) technology or carbon dioxide removal (CDR) to help make it more affordable and appealing for large-scale implementation?

A Some people argue against admitting that CDR should be part of the solution because it is interpreted as giving more life to fossil fuels. I think that's completely the wrong way to look at it. The right way to look at it is to recognize net-zero economywide emissions as just one milestone on the way to net-negative emissions, and it's a tautology that you can't do net-negative if you don't have negative carbon technologies. The more that one can develop, demonstrate, and deploy these technologies now, the more we're getting a leg up to the place where we really want to go in the future, and of course at the same time, it's going to help us with the mitigation challenge along the path to net-zero.

We've been advancing quite strenuously this carbon dioxide removal agenda, and it's getting a lot of traction. The energy bill that was attached to the Omnibus Appropriations Bill and signed by the former president on December 21, 2020, provided a lot of support for these technologies. This includes the support of a broad research portfolio on the topic and also requires a cross-administration CDR committee. The energy bill also authorized six big CCUS demonstration projects. Moving those forward will be very important, but where I think the government has to come in in a new way is to also be looking at the simultaneous buildup of the infrastructure to service these areas.

In this decade, we could start with a set of discrete hubs to advance the infrastructure of CCUS, CDR, and hydrogen, and the federal government can play a huge role in getting that to happen in collaboration with cities, states, and regions nationwide.

Turner Jackson, MITEI

MIT Energy Initiative Members

MITEI Founding and Sustaining Members

MITEI's Founding and Sustaining Members support "flagship" energy research programs and projects at MIT to advance energy technologies to benefit their businesses and society. They also provide seed funding for early-stage innovative research projects and support named Energy Fellows at MIT. To date, members have made possible 192 seed grant projects across the campus as well as fellowships for more than 500 graduate students and postdoctoral fellows in 20 MIT departments and divisions.

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COMMONWEALTH FUSION SYSTEMS

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MITEI's Associate Members support a range of MIT research consortia, education programs, and outreach activities together with multiple stakeholders from industry, government, and academia. In general, these efforts focus on near-term policy issues, market design questions, and the impact of emerging technologies on the broader energy system.

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MITEI Affiliates are individual donors and foundations that support MITEI's energy- and climate-related activities across the Institute. Specific programs include the Undergraduate Research Opportunities Program, supplemental seed funding for early-stage innovative research projects, the MIT Energy Conference, the MIT Tata Center for Technology and Design, and the MIT Climate CoLab.

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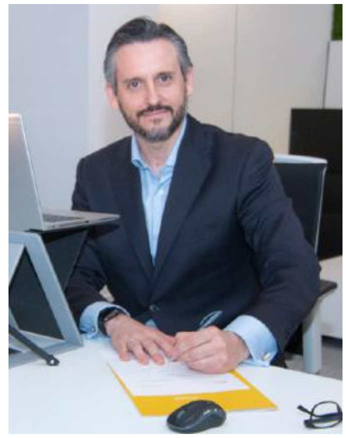
MITEI member news




Ferrovial renews MITEI membership

The MIT Energy Initiative (MITEI) has renewed its collaboration with international infrastructure company Ferrovial. The company has extended its status as an Associate Member of MITEI and will invest $5 million over the next five years to support low-carbon energy and sustainable infrastructure research at MIT. The research collaboration with MITEI has benefited projects in areas including building energy technologies, software automation for identifying energy service opportunities, uses for brine byproducts from seawater desalinization, sustainable urban mobility, and more. Ferrovial will also continue its membership in MITEI's Mobility Systems Center, which continues the multidisciplinary research started under the three-year Mobility of the Future study. Above: Dimitris Bountolos (left), Ferrovial's chief information and innovation officer, and Robert Armstrong, MITEI's director, participate in a virtual signing ceremony to renew the collaboration.

Photo of Dimitris Bountolos: ©Ferrovial
Photo of Robert Armstrong: Debbie Armstrong

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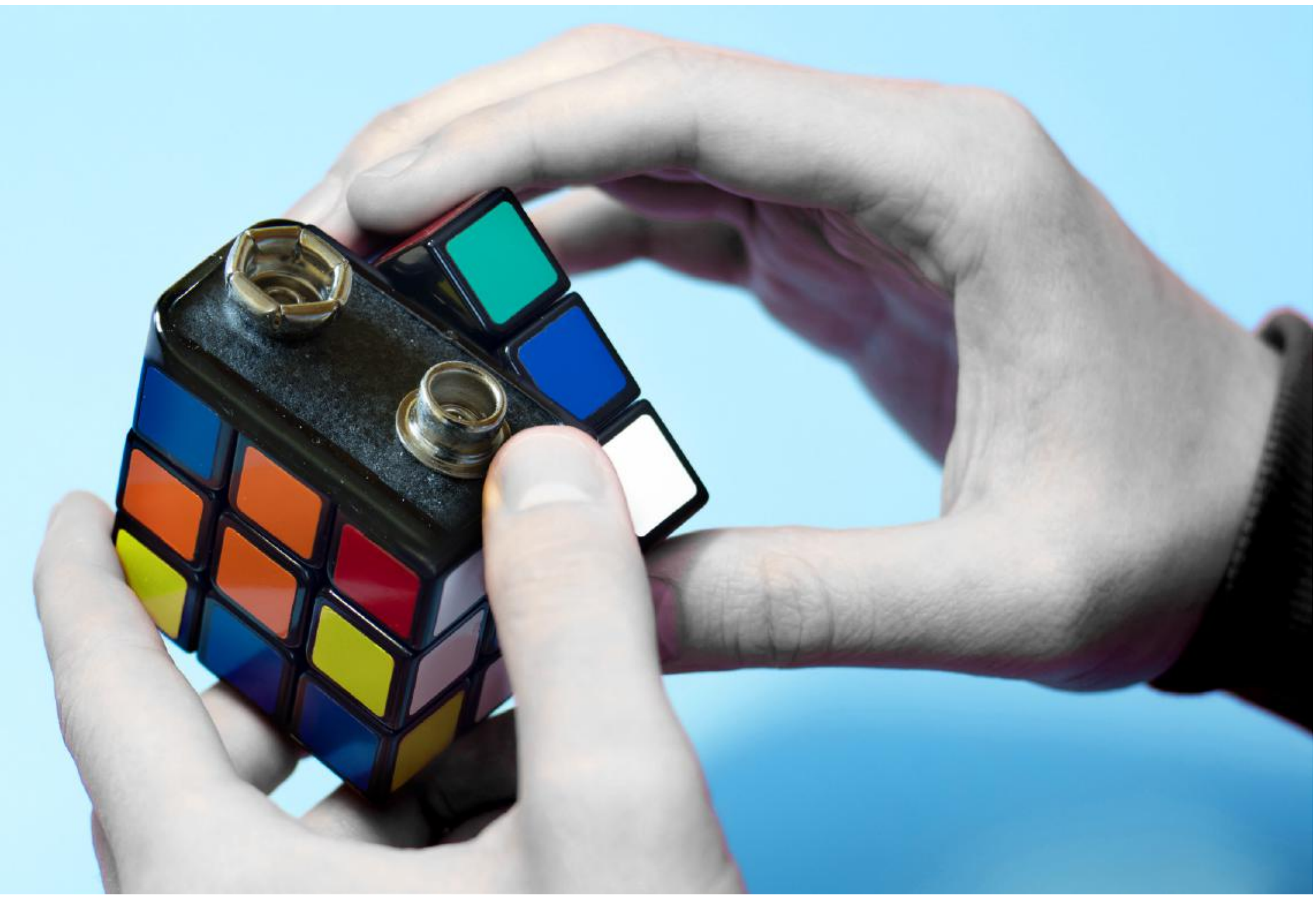

Puzzling out long-duration storage for the energy transition

Securing a carbon-free electric grid will require energy-storage technologies that can complement the variable output of renewables, storing and discharging electricity as needed over days and even weeks. MIT and Princeton University researchers explored a wide range of possible variables in the storage design space under different low-carbon grid scenarios and identified parameter combinations that could deliver innovative, low-cost, long-duration energy storage. Their analysis shows that large storage systems could potentially lower electricity cost by as much as 40% on a reliable carbon-free grid. The analysis identifies economic and technical performance targets that can help guide current efforts to develop promising long-duration storage technologies. Read more on page 25.
Photo illustration: Bumper DeJesus/Andlinger Center for Energy and the Environment, Princeton University