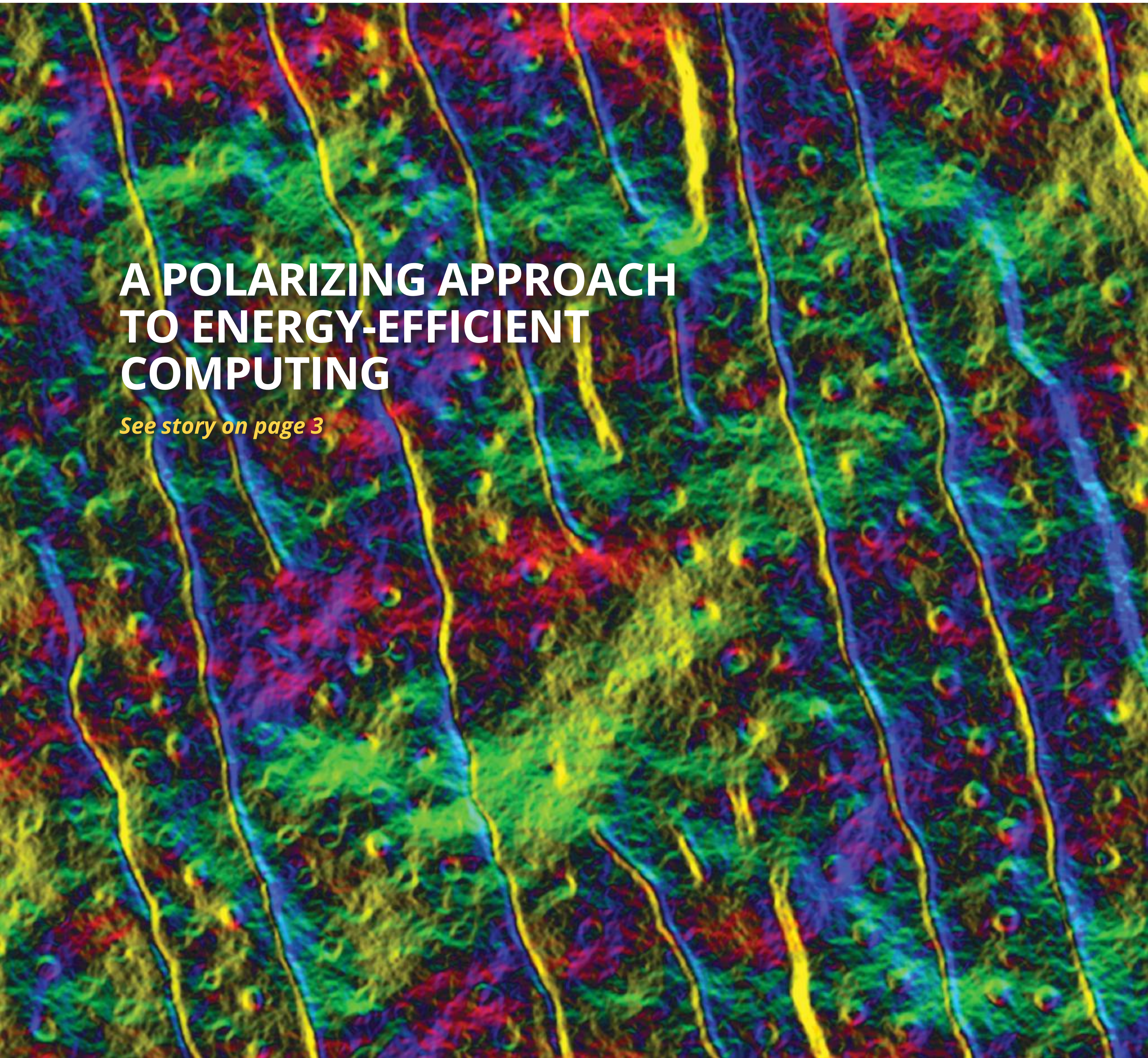
MSE NEWS

MATERIALS SCIENCE AND ENGINEERING

SPRING 2019

Carnegie Mellon University



A POLARIZING APPROACH TO ENERGY-EFFICIENT COMPUTING

See story on page 3

A NOTE FROM THE DEPARTMENT HEAD
Gregory S. Rohrer
W.W. Mullins Professor

Greetings to our MSE alumni! I am happy to report that the Department continues to grow and thrive. As always, you will find this issue of *MSE News* packed full of the successes of our students, faculty, and alumni.

MSE organizes its research into four thematic areas:

- Computational materials science
- Soft, nanostructured, and bioactive materials
- Manufacturing and materials microstructure
- Inorganic functional materials

There are, of course, overlaps between these areas — as well as some indistinct boundaries. Nevertheless, we find it useful to present our efforts to the outside world in this way.

The cover story of this issue of *MSE News* is from the area of inorganic functional materials. Within this area, Department faculty are focusing on magnetic and electronic materials for applications in information technology — including data storage, memory, and computing.

As part of this effort, a group of faculty is exploring magnetic materials for memory and computing that leverage emerging interfacial interactions associated with metals that have a strong spin-orbit interaction. Specifically, **Professor Vincent Sokalski** is leading a $1.8 million DARPA grant on domain wall skyrmions, which are magnetic excitations in metallic materials that can be moved with very little energy — compared to moving electrons, as in current devices.

Of course, there is a range of exciting research in this and other areas being carried out today in the Department of Materials Science and Engineering. In this newsletter, you will find stories about new drug release materials, high entropy alloys, materials for more efficient electric motors, quantum dots for electronic displays, and self-healing materials.

As always, *MSE News* also features many stories about recent recognition earned by our faculty, students, and alumni. Of special note, **Professor Elizabeth Holm** has been elected a Fellow of TMS. This is a highly selective designation held by three of our current faculty.

I hope you enjoy reading about the other activities and achievements of MSE faculty, alumni, and students. Please let us know of any significant developments in your career and life that we can feature in the Alumni News section.

As always, if you are in town and have the opportunity, you are welcome to visit the Department.

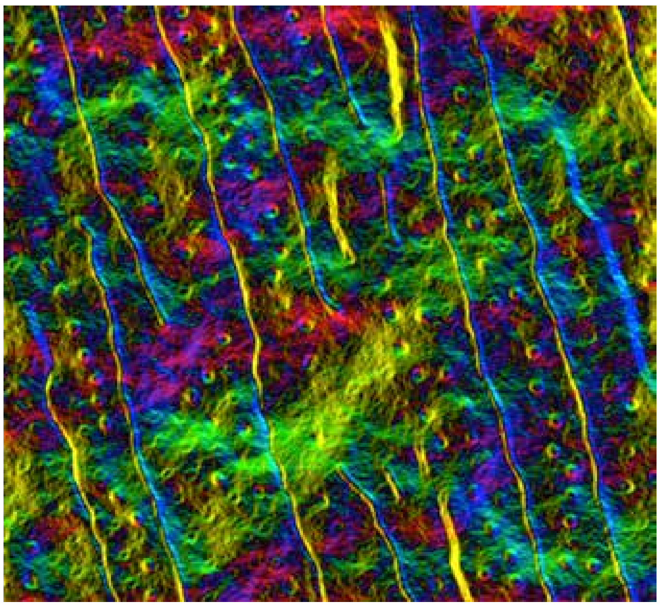
GREGORY S. ROHRER

A Polarizing Approach to Energy-Efficient Computing

Professor Vincent Sokalski *(M.S. 2009, Ph.D. 2011)* is working to address a critical worldwide issue: By 2040, society's demand for computing energy alone could exceed the global energy supply.

"More and more data is being created and moved around in our increasingly digitized world, which consumes a lot of energy," explains Sokalski, noting that many researchers believe the trend in growing computer power predicted by Gordon Moore in 1965 is nearing an end. "It's been said for some time that Moore's Law — which has been sustained by semiconductor, or silicon, technology — is reaching a fundamental limit. We are at a point where radical ideas need to be considered."

In his MSE research lab, Sokalski and his team are exploring magnetic materials that leverage a fundamentally new quantum interaction to stabilize something called a skyrmion, which he hopes could form the basis for future computer memory.



The cover image was taken with a transmission electron microscope using a technique that is sensitive to nanometer-scale magnetic features. It was produced in the Materials Characterization Facility by MSE Ph.D. student Maxwell Li. As the electron beam used for imaging is deflected by the magnetic structure of the sample, researchers can reconstruct the local magnetic orientation, which is indicated by the color. By illuminating this magnetic orientation, scientists can identify which materials are able to host skyrmions to support future computing needs.

While magnetic materials are already used in hard disk drives, they are not yet an integral part of a computer's random access memory (RAM), or central processor, where much of the energy is consumed. Sokalski hopes his lab can develop the materials needed to change that. One approach is to use skyrmions in neuromorphic, or "brain-inspired," computing for artificial intelligence.

How important is this research? Sokalski recently received a $1.8 million grant from the Defense Advanced Research Projects Agency (DARPA) for his project, "Domain Wall Skyrmions: Topological Excitations Confined to 1-D Channels." His CMU collaborators include his doctoral students **Maxwell Li, Michael Kitcher**, and **Nisrit Pandey**; MSE's own **Professor Marc De Graef**; Professor Di Xiao from the Department of Physics; and Physics student Caitlin Carnahan. Tim and Claudia Mewes from the University of Alabama Physics Department are also collaborating on the grant.

"DARPA actually created a new program called 'Topological Excitations in Electronics' to fund projects that improve magnetic materials used for computer memory and processors," notes Sokalski. "It's a challenge for both civilian and military technology applications. One benefit of magnetic memory is that it is not susceptible to fluctuations in available power sources, which could be valuable for supporting military operations in remote areas."

So how does the technology work — and how does it contribute to greater energy efficiency?

"In magnetic materials, each electron has a natural magnetic dipole called spin," says Sokalski. "Think of it as an arrow. In most magnetic materials, like a bar magnet, these arrows are aligned in the same direction, giving us the well-known north and south poles."

"But with certain new materials, these arrows can instead form exotic swirling patterns called skyrmions, which are a highly mobile kind of vortex — think of a tornado — but now only a few billionths of a meter in size," he continues. "They can fit into smaller spaces with the digital data encoded by their positions. Skyrmions can also be moved around with a small amount of energy, making them ideal candidates for energy-efficient computing."

"The biggest challenge is discovering materials that have the right properties needed for skyrmions to be stable. Ultimately, it's a matter of understanding and then capitalizing on a naturally occurring phenomenon that occurs in certain magnetic materials," Sokalski concludes. "It may just represent a nanoscale solution to a large-scale global problem."

Sokalski and Skyrmions

Bettinger Awarded Patent

Bettinger's next-generation extended-release capsule relies on a battery that will eventually lose its charge — releasing the medication.

After years of research, **Professor Christopher Bettinger** has patented a unique ingestible capsule that can deliver medicine to the hard-to-reach lower part of the digestive tract. The capsule, made of plastic or a non-toxic material, is filled with medicine through a small hole, capped with a film of metal, and wired with a battery. When the precisely timed battery charge runs out, the film dissolves and the medicine is released. In October 2013, Bettinger completed his patent application for an "ingestible, electrical device for oral delivery of a substance" — and the patent was awarded in February 2018. This innovation solves the problem of trying to deliver medicine in an extremely targeted manner to the lower intestinal tract. Traditional large capsules tend to dissolve before reaching there, and the process is not exact — making it impossible to predict the outcome and the amount of medicine actually delivered. Bettinger, who holds a joint appointment in MSE and Biomedical Engineering, has also co-authored a paper in *Advanced Functional Materials* on yet another innovation: soft, adhesive hydrogels that can function as brain-machine interfaces due to their compatibility with brain tissue. When printed with tiny electrode arrays, these gels can help patients manage pain, control seizures, and interact more effectively with the external world.

Marom Chosen for Exascale Computing Program

Professor Noa Marom has been selected to lead one of 10 data science projects as part of the Argonne Leadership Computing Facility's (ALCF) Aurora Early Science Program (ESP). Set to be the first exascale computing system in the US when it is launched in 2021, Aurora will have the computing power to perform a quintillion calculations per second. The goal of the ESP is to prepare Aurora's key applications, libraries, and infrastructure for the architecture and scale of exascale computing — while allowing universities and national laboratories to optimize their applications for the new architecture. Called "Many-Body Perturbation Theory Meets Machine Learning to Discover Singlet Fission Materials," Marom's project aims to harness exascale power to revolutionize the process of photovoltaic design to create more efficient organic solar cells. She will leverage Aurora's resources to combine quantum-mechanical simulations with machine learning and data science to advance the shared understanding of singlet fission as a source of electricity generation. Previous Early Science Program projects helped usher in earlier ALCF supercomputers, including the Intel-Cray system Theta and the IBM Blue Gene/Q system Mira, both of which continue to serve the scientific research community today.

Webler and Collaborators Win MFI Award

Professor Bryan Webler is part of a collaborative Carnegie Mellon team that has won a Manufacturing Futures Initiative (MFI) award from the University. Along with fellow researchers Maarten de Boer (Mechanical Engineering) and Barnabas Poczos (Machine Learning), Webler is developing high-entropy alloys, a new class of metal alloy. All three researchers are affiliated with CMU's additive manufacturing research center, the NextManufacturing Center. They will synthesize their high-entropy alloy laboratory specimens using additive manufacturing methods. While traditional alloys are made up of one base metal, high-entropy alloys are composed of metals all in roughly equal concentrations. These alloys may perform better than traditional materials used in high-temperature applications such as aerospace power generation, where they show promise to resist damaging chemical reactions such as oxidation. Because high-entropy alloys are complex and expensive to produce, it is impractical to make entire structures from them. Instead, Webler and his collaborators will investigate coating structures with the new materials, making overall structures more durable at a lower cost.

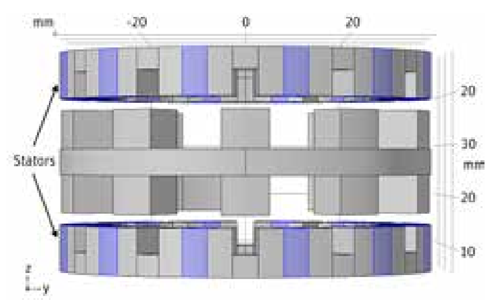
Webler and the MFI Award

Cohen-Karni Receives Early Career Fellowship

Professor Tzahi Cohen-Karni recently received the CIT Dean's Early Career Fellowship from the College of Engineering. Dean's Early Career Fellowships are awarded to untenured faculty members who have been nominated by their department heads and then selected to receive the fellowship after review and discussion of the nomination package by the CIT Review Committee. Recipients receive discretionary funds for a three-year period, or until such time when they have been promoted to full professor. With a joint appointment in MSE and Biomedical Engineering, Cohen-Karni studies the synthesis and utilization of nanomaterials, and the creation of three-dimensional hybrid nanostructures from Si and Ge nanowires and two-dimensional graphene. He has previously received the NSF CAREER Award, ONR and Charles E. Kaufman Foundation Young Investigator Awards, and Cellular and Molecular Bioengineering Young Investigator and Rising Star Awards.

McHenry Develops Next-Generation Motor

Statistics show that 50 percent of energy in the US goes through a motor — from cars and planes to refrigerators and industrial machines. **Professor Michael McHenry** is leading the development of a revolutionary new motor technology that uses soft magnetic materials to increase efficiencies to exceed 96 percent, which could significantly impact energy usage and efficiency across a wide range of applications. When a motor operates to transform electrical energy to mechanical energy, an alternating current provides a magnetic field to the magnetic materials inside the motor. The magnetic dipoles then switch from north to south, and cause the motor to spin. However, current silicon steel materials heat up during this process, which negatively impacts energy production. McHenry is replacing these steels with next-generation metal amorphous nanocomposite materials (MANCs) — a class of soft, magnetic materials that are efficient at transforming energy at high frequencies. By applying this technology, motor designs can shrink as they deliver the same output — or outputs can dramatically increase as the motor size remains the same. McHenry's research group in MSE is collaborating with the National Energy Technology Laboratory (NETL), NASA Glenn Research Center, and North Carolina State University to design and test motor designs, with funding from the Department of Energy (DOE) Advanced Manufacturing Office.

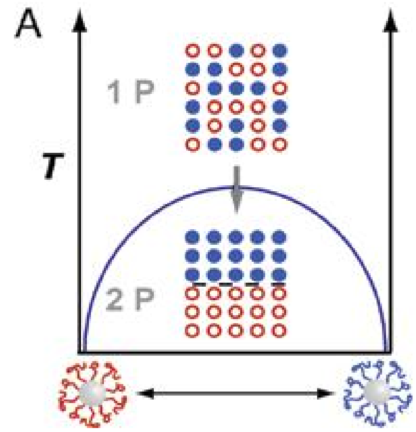


Dual stator design for a motor with gray representing CMU patented metal amorphous nanocomposite materials (MANCs) and the blue is rare-earth free permanent magnet materials.

McHenry's magnetic materials

Bockstaller Receives DOE Grant

Professor Michael Bockstaller recently was awarded funding from the US Department of Energy's Basic Energy Sciences (DOE-BES) program. This grant, worth $1.1 million over three years, will support Bockstaller's collaborative work with researchers at the University of Houston to understand the organizational behaviors of nanoparticles like quantum dots. These materials are integral to the quality of image display technology. If Bockstaller and his collaborators can understand and control the parameters that cause these quantum dots to form into organized structures — for example, how they group according to color — their research may be able to dramatically improve the resolution of electronic displays and optical devices. Specifically, the team will attach polymer chains to the particles' surface and study the effects of this process on particle behavior. They have already observed that the attachment of polymer chains causes nanoparticles to separate and re-assemble; now they need to understand the driving forces behind this activity.



If Bockstaller and his fellow researchers can drive particles to autonomously organize by color, they can significantly improve image resolution for electronic and optical devices.

Bockstaller's DOE-BES grant

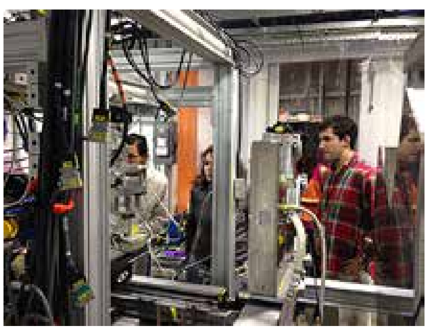
Holm Named TMS Fellow

Professor Elizabeth Holm has been inducted as a 2019 Fellow of The Minerals, Metals & Materials Society (TMS). The Society named just nine Fellows for 2019. Holm's citation reads, "For pioneering achievements and leadership in computational materials science and Integrated Computational Materials Engineering and for distinguished service to the materials profession." The highest honor given by TMS, this award recognizes members of TMS who have made outstanding contributions to the practice of metallurgy, materials science, and technology. This includes scholarship, such as the publication of articles or books; the granting of patents; direction of important research or engineering work; and responsibility through management for nationally known improvements and developments in the field. In her research at MSE, Holm uses the tools of computational materials science to study a variety of materials systems and phenomena. Her research areas include the theory and modeling of microstructural evolution in complex polycrystals, the physical and mechanical response of microstructures, mechanical properties of carbon nanotube networks, atomic-scale properties of internal interfaces, machine vision for automated microstructural classification, and machine learning to predict rare events.

Islam Shares in MFI Grant

Professor Mohammad Islam recently received a grant from Carnegie Mellon's Manufacturing Futures Initiative (MFI) in partnership with **Lining Yao**, a faculty member at the Human-Computer Interaction Institute in the School of Computer Science. Yao holds a courtesy appointment in MSE. Islam and Yao are collaborating to develop synthetic materials that repair themselves over time, just as the human body recovers from a cut or a sprain. The team's unique actuator, called Healer, is expected to fully heal itself within a few hours with the same shape, functionalities, and properties as before if it is broken into pieces. Such actuators can be used as sensors and synthetic muscles. Using 3D printing technology, Islam and Yao plan to fabricate an actuator by printing conductive self-healing polymer composites in a layer-by-layer process. The actuator will have embedded pores, filled with liquid, that allow it to expand and contract like a muscle when heated up or cooled down. The MFI grant will enable Islam and Yao to both develop the material and raise the scale of its production. Launched in 2017, CMU's Manufacturing Futures Initiative supports interdisciplinary research aimed at accelerating the maturation of new materials and process discoveries, while also helping to stimulate economic growth in the Pittsburgh region.

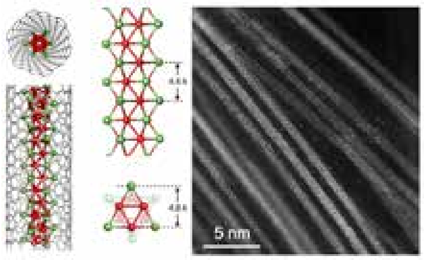
Rollett Seeks Answers to 3D Printing Challenges



Carnegie Mellon researchers are shown at work in the Argonne National Labs Advanced Photon Source facility.

[Keyholes in metal 3D printing]

Anthony Rollett, an MSE professor and Co-Director of CMU's NextManufacturing Center, recently co-authored a paper with his own research team and scientists from Argonne National Laboratory. Called "Keyhole Threshold and Morphology in Laser Melting Revealed by Ultrahigh-Speed X-Ray Imaging," the paper appeared in *Science* in February. The collaborative team is seeking answers to a pressing issue that stands in the way of large-scale 3D printing: Why do tiny gas pockets often appear in the final product, leading to cracks and other failures? Rollett and his co-authors are elucidating how and when these gas pockets form, as well as a methodology to predict their formation — a pivotal discovery that could dramatically improve the 3D printing process. The scientists used the extremely bright, high-energy X-rays at Argonne's Advanced Photon Source (APS), a Department of Energy Office of Science User Facility, to take super-fast video and images of a process called Laser Power Bed Fusion (LPBF), in which lasers are used to melt and fuse material powder together. By watching what happens as the laser moves across the metal powder bed to create each layer of the product, the team observed an effect called "keyholing" which can lead to materials defects. By understanding and addressing this phenomenon, the CMU-Argonne researchers are solving one of the most fundamental problems associated with additive manufacturing.



Shown here is a graphical rendering of the crystal structure of the material Shukla synthesized—a stack of alternating triangles of Molybdenum (red) and Tellurium (green), forming a transition metal monochalcogenide nanowire inside a carbon nanotube. On the right is a STEM (scanning transmission electron microscope) image of the actual material sample.

Junior **Shivani Shukla** is the co-first author of a paper accepted for publication in the technical journal *ACS Nano Letters*. In addition, an image published by Shukla will appear on the journal's cover when it is printed this August. The paper is the outcome of Shukla's Nakatani-RIES Fellowship in the Department of Chemistry at Nagoya University in Japan following her freshman year. She conducted research and testing to incorporate new materials with specific electrical properties into carbon nanotubes. The paper, called "Isolation of Single-Wired Transition-Metal Monochalcogenides by Carbon Nanotubes," reflects her findings, along with other researchers. A dual major in MSE and BME, Shukla plans to pursue a Ph.D. and continue her work as a researcher following graduation.

MSE Ph.D. candidate **Andrew Kitahara** recently wrote a guest column for the International Metallographic Society's (IMS) newsletter called "Sliplines." Kitahara was elected as the IMS Student Board Member for 2019. As the Student Board Member, Kitahara receives paid travel expenses to attend and actively participate in all IMS Board meetings. He serves as the voice of students nationwide and takes an active role in shaping the future of the International Metallographic Society. Advised by **Professor Elizabeth Holm**, Kitahara is focusing his MSE thesis on applied computer vision techniques for augmented and autonomous microscopy.

Senior **Dominique Petach** has been selected as a Perryman Scholar for the 2018-19 school year by the Perryman Family Foundation. Petach, who is a double major in MSE and Biomedical Engineering (BME), was recommended for the scholarship by BME Professor Conrad Zapanta and CMU Dean of Student Affairs Gina Casalegno. Following her graduation this spring, Petach's educational goal is to pursue a masters in BME at Carnegie Mellon. She is also considering earning a doctorate in biomedical engineering.

Three MSE Students Named ACS Scholars

Three seniors in the Department of Materials Science and Engineering have been selected as 2018-19 Andrew Carnegie Society (ACS) Scholars. These students are **Mari-Therese Burton**, as well as **Gaurav Balakrishnan** and **Jack Forman**, both dual majors in MSE and Biomedical Engineering (BME). *(Editor's note: See story on Forman on page 9.)*

ACS Scholars are undergraduate seniors who embody Carnegie Mellon's high standards of academic excellence, volunteerism, leadership and involvement in student organizations, athletics or the arts. They are selected each year by their deans and department heads to represent their class in service and leadership.

< Shown left to right are ACS Scholars Jack Forman, Mari-Therese Burton, and Gaurav Balakrishnan.

Fashioning a Unique Career Path

Senior Jack Forman aims to redefine the idea of "wearables" by custom-designing functional materials for clothing

What leads someone to become a materials scientist? For senior **Jack Forman**, it began when he read Roald Dahl's *Charlie and the Chocolate Factory* as a child. "There were these incredible inventions, like edible wallpaper," he recalls. "I was enthralled that there could be materials with these crazy properties — but then disappointed to learn they didn't actually exist."

As a high school junior, Forman built on his interest in materials by taking a summer workshop in nanotechnology at the University of Pennsylvania. "We learned about color-changing, stretch-responsive paint, and carbon nanotubes that could be used to make an elevator to space — and I thought, 'This reminds me of Willy Wonka's candies and glass elevator.' I knew then that I wanted to be a materials scientist," he says.

Forman enrolled at CMU because of its strong dual focus on science and art. "I've always considered myself a creative person," notes Forman. "As a materials scientist, I wanted to collaborate with artists and designers. CMU is the perfect environment for that."

Forman's materials innovations are aimed at combining form with function.

The Art and Science of Design

Chief among Forman's collaborators is **Professor Lining Yao** of the Human-Computer Interaction Institute in the School of Computer Science, who holds a courtesy appointment in MSE. In his junior year, Forman joined Yao's Morphing Matter Lab, focused on materials that change properties.

Under Yao's guidance, Forman co-designed a clothing line for CMU's 2018 Lunar Gala student fashion show. Along with fellow MSE senior **Alan Guo** and Costume Design graduate student Mohan Yeh, Forman developed clothing that responds intelligently to temperature. Explains Forman, "A jacket can get puffier in colder weather, or sleeves can roll up automatically as the ambient temperature increases."

The clothing incorporates a unique silver-coated nylon thread, ModiFiber, that functions as an artificial muscle — expanding and contracting, or twisting and untwisting, in response to heat.

While Yao gave Forman a qualitative perspective on design, **Professor Robert Heard** and other MSE faculty provided the quantitative science. "Professor Heard's 'Selection and Performance of Materials' course taught me that, if an object is to thrive in its function, the ideal properties need to be defined and weighted," Forman points out. "Then the materials can be selected according to the properties — such as Young's Modulus or yield strength — that deliver the best performance."

"Both modes of thinking are critical," he continues. "Engineering design allows me to make products that function well, and artistic design ensures those products will inspire and excite."

In May, the clothing line will be shown in Moscow, Russia, at the State Historical Museum's competitive global event, called "Innovative Costumes of the 21st Century: the Next Generation." Also in May, Forman will present his work on ModiFiber at CHI '19, the world's most prestigious conference for human-computer interaction, in Glasgow, Scotland.

Following graduation, Forman plans to attend the Program in Media Arts & Science at MIT Media Lab, which facilitates the creative application of digital technologies. Eventually, he would like to lead his own lab. "My goal is to remind people that the physical world, and our interaction with it, is magical," notes Forman. "I want to combine the best of digital interaction with the best of tangible interaction to create entirely new experiences."

[Jack Forman and adaptive clothing]

Revealing the Secrets of the Cell

Biophysicist and MacArthur Fellow Cliff Brangwynne (B.S. 2001) studies the materials science of biological organization

Clifford Brangwynne *(B.S. 2001)* — a professor in Chemical and Biological Engineering at Princeton University — has traveled an impressive path since his graduation from Carnegie Mellon. His work to elucidate the fundamental principles underlying biological organization, especially how membrane-less organelles form within living cells, has attracted attention for its potential to increase the shared understanding of disease mechanisms.

"My research focuses on revealing how these membrane-less structures form, what can go wrong in their assembly, and how that might contribute to diseases like cancer and Alzheimer's," Brangwynne explains. "The biophysical processes that lead to disease are still not well understood, so this is an emerging field of study that could have huge implications."

Brangwynne's groundbreaking work has been recognized with a number of awards, including a New Innovator Award from the National Institutes of Health in 2012, a Searle Scholar Award in 2012, a National Science Foundation CAREER Award in 2013, and a Sloan Research Fellowship in 2014. Last year, he was appointed an Investigator of the Howard Hughes Medical Institute at Princeton.

Also in 2018, Brangwynne was named one of 25 MacArthur Fellows by the John D. and Catherine T. MacArthur Foundation, which strives to support transformative change in pressing areas such as global climate change and nuclear risk.

According to a statement released by the MacArthur Foundation, these 25 individuals were chosen for their efforts in "solving long-standing scientific and mathematical problems, pushing art forms into new and emerging territories, and addressing the urgent needs of under-resourced communities. Their exceptional creativity inspires hope in us all."

Brangwynne was selected alongside a diverse group of individuals that includes other scientists, but also writers, artists, filmmakers, community organizers, and social advocates. "This is a unique honor because it acknowledges that scientists are making important contributions to improving the human condition — and it elevates our work," he notes. "I was completely surprised by my selection, as the MacArthur Foundation keeps the nomination process very secretive."

A Crystalizing Moment at MSE

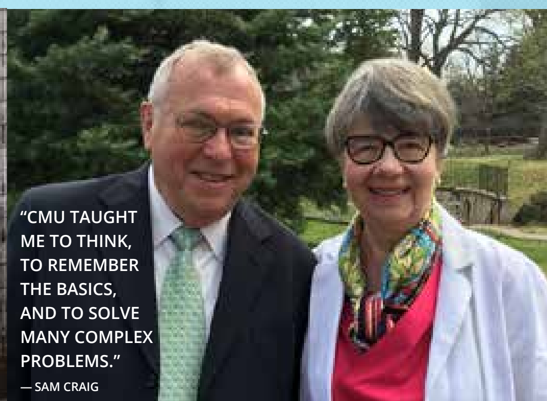
Ironically, Brangwynne initially enrolled in the College of Humanities and Social Sciences as a CMU freshman. But after a serendipitous conversation with an MSE doctoral student back home in Boston, Brangwynne signed up for "Introduction to Materials Science and Engineering" — and was immediately hooked.

"In a lab session, we heated a metallic alloy to over 1000 degrees and then examined the grain structure," Brangwynne recalls. "I still remember being completely awestruck as I watched the process of atomic crystallization happening. It was amazing, and it convinced me to declare my major in MSE."

Brangwynne went on to earn a Ph.D. in 2007 in Applied Physics at Harvard, followed by a three-year stint as a postdoctoral researcher at the Max Planck Institute of Molecular Cell Biology and Genetics and the Max Planck Institute for the Physics of Complex Systems. He joined the Princeton faculty in 2011.

While Brangwynne now focuses on biophysics as opposed to more traditional topics in materials science, he still sees a direct connection to his roots at Carnegie Mellon. "At CMU, I studied the principles of phase transformation in materials, and I am still focusing on how phase transformations occur — only now in living cells," he points out.

Clifford Brangwynne and the MacArthur Fellowship



SAM CRAIG 1957

Give strategically, Support generously.

SAM CRAIG (EE '57, '58, '61) used his engineering background to build a diverse career. He has made an impact on a number of fields through his research in industry, projects in noise reduction, and work in product design in the healthcare industry. He joined the engineering faculty at Bucknell University where he continues to teach at Bucknell's Institute of Lifelong Learning.

For Sam and his wife Nancy Owen Craig, Carnegie Mellon University has always been an important part of their philanthropic life because of the pride they feel for the continued success of the Department of Electrical Engineering (ECE).

Sam and Nancy have created a lasting legacy at Carnegie Mellon by establishing a life income plan and an annuity that will both provide scholarship support for undergraduate students in ECE. The scholarships were created in honor of Sam's parents.

Learn how easy it is to achieve your philanthropic vision through a planned gift by visiting giftplanning.cmu.edu. Contact the Office of Gift Planning today at 412.268.5346 or askjoebull@andrew.cmu.edu.

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