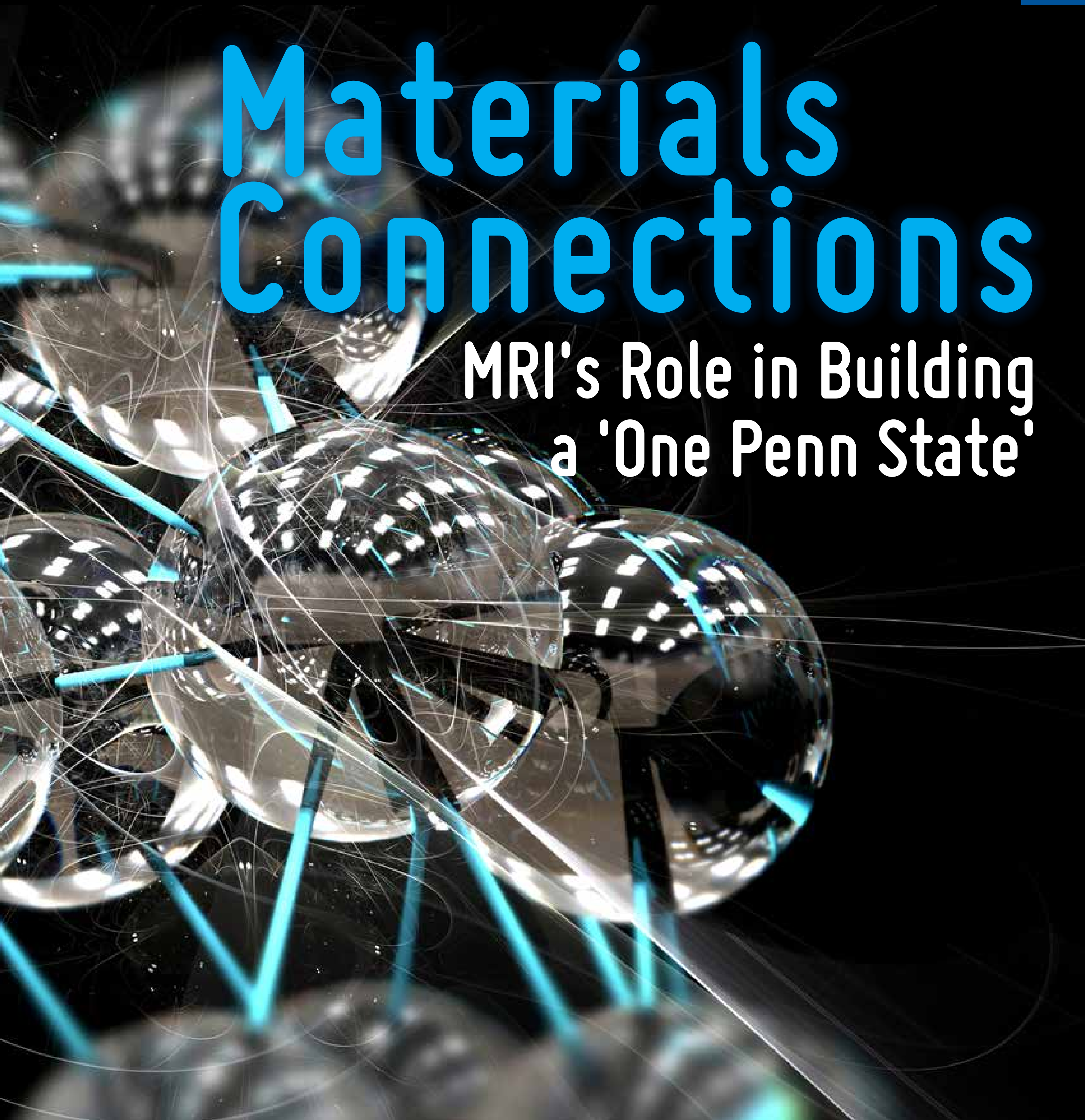
PennState
Materials Research Institute

FOCUS on MATERIALS
MATERIALS RESEARCH INSTITUTE BULLETIN

SPRING 2022

Materials Connections

MRI's Role in Building a 'One Penn State'



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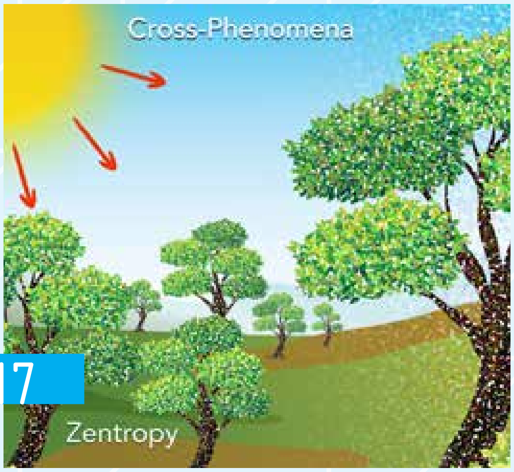

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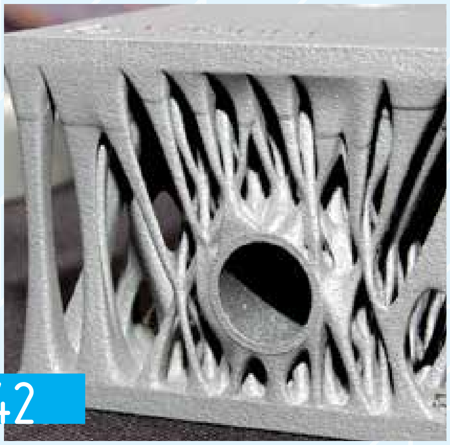

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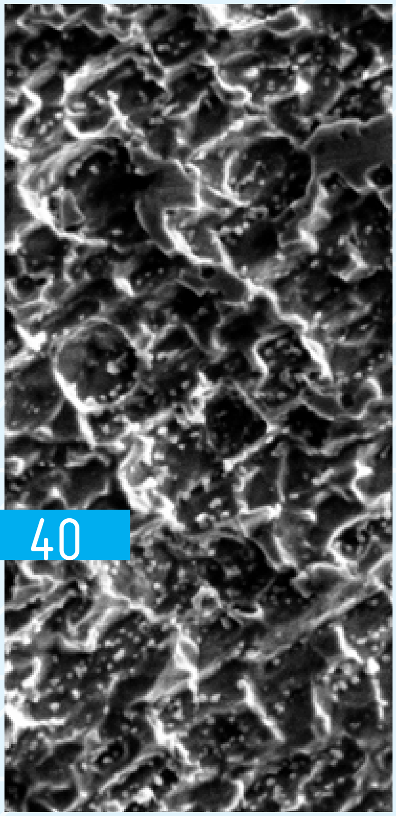

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Focus on Materials is a bulletin of the Materials Research Institute at Penn State University. Visit our web site at **www.mri.psu.edu**.

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From the Director

Penn State has a culture of embracing interdisciplinary research to address complex programs and challenge itself with expanded dialogue. The University's history of interdisciplinary research goes back even to the times of Elburt Osborn as vice president for research in the late 1940s. In fact, his philosophy led to the inspiration of others to develop the first interdisciplinary research laboratory in the nation which was the materials research lab under the leadership of Rustum Roy in the 1960s!

We in the Materials Research Institute continue to strive with this tradition by building a community of materials research that spans our entire research ecosystem, crossing campuses, colleges, departments, and institutes. This issue of Focus on Materials offers you, the reader, just some of the many interdisciplinary success stories we can tell.

This interdisciplinary materials community was built over several years by enabling a system that allows the maximum number of people to come together. From an MRI perspective, the best way to create such a gathering of researchers is through our core facilities. Our facilities, such as the 2D Crystal Consortium, the Nanofabrication Lab, and the Materials Characterization Lab, provide Penn State researchers with state-of-the-art equipment and expert staff. These core facilities then act as a platform for collaboration among many different researchers, both within materials and sometimes, outside of materials.

All our efforts run in parallel with the overall Penn State philosophy of collaborative research, as is evident by the University's interdisciplinary research institute system. There are seven of these institutes, of which the Materials Research Institute is one. This is also in parallel with One Penn State 2025, an initiative started in 2021 to create a seamless, diverse, and interdisciplinary learning experience.

Our interdisciplinary approach allows us to launch productive risky ideas, such as ideas we love to entertain in our seed grant programs. We promote our seed grant program to encourage collaborations among partners outside of their own units to explore innovative ideas for transformative, high-impact materials research. This year, 18 grants were awarded by MRI in partnership with Penn State's Applied Research Laboratory, College of Medicine, Huck Institutes of the Life Sciences, and the Pennsylvania Recycling Markets Center in Harrisburg, Pennsylvania. We offered grants in strategic areas such as quantum, sustainable materials, convergent science, data science, and many others. It was fantastic that colleges and our fellow institutes partnered with us in areas where there was overlap, so these seed grants encouraged people to form new teams and work together across the University.

Those types of seeded programs are often a step toward testing proof of concepts, enabling compelling data to support faculty in terms of grant submissions. For example, Penn State did very nicely in this last round of Multidisciplinary University Research Initiatives grants from the Department of Defense. For instance, the group led by our MRI colleague Rongming Chu submitted a winning proposal, "Effects of Radiation Damage on Performance of Wide-Bandgap Electronics" that featured a team of faculty from both the Penn State University Park and Behrend campuses. It is a particularly good example of how we can operate as a "One Penn State" research community.

Moving forward, Penn State's interdisciplinary methodology gives us a leg up as our society's issues grow more complex and urgent, and require us to think beyond the STEM subjects. Indeed, we are seeing that sophisticated problems like pandemics and climate change require perspectives from social scientists, artists, and many other areas that were completely ignored in materials before. We in MRI are exploring that new frontier as well, as there are always new ideas and challenges coming. All said, it is inspiring to think about where our One Penn State Materials Research Community may go next, and what impact our work may have.

Sincerely,

C A Randall

Director, Materials Research Institute

IN TOUCH WITH ESTHER OBONYO: BUILDING SUSTAINABLE, SAFE, GLOBAL COMMUNITIES

By Samantha Chavanic

IN 2015, ALL United Nations member states adopted the 2030 Agenda for Sustainable Development — a blueprint outlining 17 Sustainable Development Goals focused on peace and prosperity around the world.

Esther Obonyo, associate professor of engineering design and architectural engineering, leads the Global Building Network, an initiative of Penn State and the U.N. Economic Commission for Europe aimed at advancing building science, construction, and management to accomplish Sustainable Development Goal 11: Sustainable Cities and Communities. Obonyo also serves as the lead for a $1.1 million Belmont Forum-supported consortium working to improve resilient and sustainable housing in low-income communities impacted by climate change.

In this Q&A, Obonyo speaks with Penn State engineering writer Samantha Chavanic about working to improve resilient and sustainable housing in low-income communities impacted by climate change.

Esther Obonyo associate professor of engineering design and architectural engineering Credit: Patrick Mansell/Penn State

Q: WHAT DREW you to the built environment?

Obonyo: I was born and brought up in Nairobi, Kenya. Even though I'm from a middle-income family, I have lots of relatives who are in the lower social-economic status. From an early age, one of the things I was painfully aware of was the inadequate supply of quality housing for the masses. In these situations, you are not only looking at issues of building performance and technology, but also issues of economy. The transdisciplinary effort required to address this complex challenge of affordable, adequate housing drew me into feeling like this is a profession that can help me contribute. ►►►

Q: HOW DOES your joint appointment in engineering design and architectural engineering embody this cross-disciplinary effort?

Obonyo: To address the challenge of affordable, adequate housing holistically and comprehensively, you need trans-disciplinary efforts. Coming to Penn State gave me an opportunity to explore synergies across multiple disciplines. I can maintain a grounding in engineering design and look at food insecurity as an aspect of adequate housing without losing credibility in the professional circles I move in, while concurrently exploring building performance aspects through my architectural engineering appointment.

Q: WHAT IS the Global Building Network undertaking in support of sustainable, safe buildings around the world?

Obonyo: The Global Building Network's design allows synergies with universities and organizations to happen organically. It's not competitive — it's about being humble and saying, 'we are great at what we do, but what we do is not going to get us there,' in terms of supplying affordable, adequate, resilient, low-income housing and decarbonizing the building sector. Translating potential solutions into scalable impact requires several institutions working collaboratively. That's what the Global Building Network is all about.

We have an opportunity to avoid potential problems through knowledge transfer. It is established fact that the bulk of new buildings will be constructed in the global south. We are worried that if the global south follows the trends of the global north, we will not achieve our targets for healthy, resilient, sustainable, low-income housing. We can also translate the lessons and experiences of the global south into strategies to use at scale in the global north, such as the use of locally resourced, low-carbon materials to inform material-related decarbonization efforts.

The final piece of the puzzle is related to human dignity and respect — housing is a basic human right. We've seen during the current pandemic that it's at the center of our health, well-being, and performance.

Q: HOW WILL you and your collaborators use the Belmont funding to improve low-income communities?

Obonyo: A priority activity for me, at a personal level, is trying to engage with governmental and non-academic stakeholders. For me, step number one is making sure all stakeholders understand the value we create as academics. We've also prioritized gathering input from community members. The lived experiences of communities should inform every phase of the research process. Understanding and addressing the unique concerns and priorities for these different stakeholders requires input from multiple disciplines.

The question we are really trying to answer is 'what causes vulnerability?' We have failed community members by proposing one-dimensional solutions — we show up, we provide the walls, roof, windows, doors. Being adequately housed is more than the physical structure. In our research, we are redefining this with the help of social scientists, trying to find ways to connect with what the household members are asking for. Is it access to food, water, energy? All these still require a physical building. We can connect these needs to bankable projects policymakers can move and influence.

Q: WHAT'S NEXT?

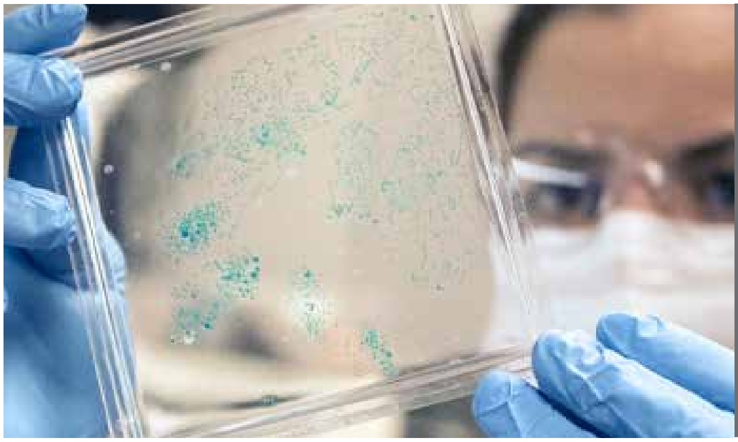
Obonyo: At the workshops and research presentations I've attended over the years, we usually end up with this statement: '… but the government." I would like the projects we are working on to have a different end, one where we say, '… and the government.' That's what's next for me — getting to the point where our research moves policymaking. ■

This story first appeared in the Fall 2021 issue of Research|Penn State magazine.

PENN STATE MATERIALS RESEARCH SHINES IN NATIONAL RANKINGS

Materials science #1, materials engineering #2 in latest NSF HERD rankings

By David Pacchioli



Credit: Patrick Mansell/Penn State

PENN STATE'S RESEARCH enterprise ranks 22nd in the country in total research expenditures, according to the latest National Science Foundation rankings of Higher Education Research and Development (HERD) research expenditures, released in January 2022.

The rankings, for the 2020 fiscal year, show Penn State rising from 23rd place in 2019. In addition, the University ranks fourth nationally in the breadth and depth of its research enterprise, as measured by the number of top-ten rankings in key fields and subfields of science and engineering. Penn State had 12 top-ten rankings for 2020. Only Johns Hopkins University, the University of Michigan, and MIT had more, with 17, 14 and 13 respectively.

The rankings do not include Penn State's Commonwealth Campuses, which together generate approximately $10 million in research expenditures.

Among the individual fields, Penn State ranked first nationally in materials science and second in materials engineering for the fourth consecutive year, demonstrating the University's exceptionally strong position in materials research.

"Our continuing success in materials science and materials engineering is built on decades of tradition, strong institutional commitment, and a unique infrastructure that encourages and enables collaboration," said Clive Randall, distinguished professor of materials science and engineering and director of the Materials Research Institute.

"On these foundations we continue to push forward to help shape the future, by enabling our faculty and students to be successful through accelerating discovery and impact. Our innovative interdisciplinary approach, coupled with the collegiality of our faculty and staff, also helps in the recruitment of new researchers to continually explore new boundaries."

Additionally, the University ranked second in mechanical engineering and psychology; fourth in electrical engineering, sociology, and total engineering; sixth in aerospace engineering and industrial and manufacturing engineering; seventh in mathematics and statistics; eighth in computer science; and 10th in atmospheric science and meteorology. Penn State also ranked No. 1 among Pennsylvania's public universities in industry sponsored research.

"Once again these rankings reflect the excellence that defines Penn State's research enterprise and sets it apart," said Lora Weiss, senior vice president for research. "The breadth and depth of our expertise is matched by the dedication and resilience of our world-class faculty. Our unique interdisciplinary approach enables us to creatively and effectively address the world's most pressing challenges." ■

PENN STATE PARTNERS WITH TWO UNIVERSITIES FOR DIVERSITY IN MATERIALS RESEARCH

By Jamie Oberdick

THE NATIONAL SCIENCE Foundation (NSF) has named Penn State the lead partner to both Florida International University (FIU) and North Carolina Central University (NCCU) as part of the Partnerships for Research and Education in Materials (PREM) program.

The PREM is funded by the NSF as a prestigious award to minority-serving institutions to increase diversity and inclusion in materials research through collaborative research projects, institutional capacity building, and student-focused educational activities with NSF centers and facilities. Its central goal of increasing recruitment, retention, and degrees earned by underrepresented groups is achieved by engaging underserved populations with opportunities for research and professional development in materials.

At Penn State, one of the PREM efforts is led by the Center for Nanoscale Science. The center is one of 19 Materials Research Science and Engineering Centers (MRSEC) in the United States funded by NSF, which bring together expertise from physical, biological, and computational sciences and engineering, for fundamental materials research. The centers also have broad portfolios of education and outreach programs that target audiences from K-12 through graduate school, as well as the general public.

The Penn State/NCCU PREM partnership features two core research thrusts linking interests and capabilities at both institutions to extend the scope and depth of research beyond those accessible at either institution. Thrust 1 focuses on mixed-dimensional (0D or 1D/2D) heterostructures for sensing, photovoltaic, and photocatalytic applications. Thrust 2 explores hybrid metal/semiconductor, organic-inorganic perovskite, and polymer/ceramic nanocomposites, and the impact of nanoscale structure on optical and dielectric properties.

The PREM research and mentoring experience provides invaluable training and experience for NCCU undergraduate and masters students looking to pursue doctoral degrees or begin careers in science, technology, engineering, and math (STEM).

Penn State Millennium Scholars and MRSEC grad students served as "Penn Pal" mentors (on the left in blue) to National Science Foundation-funded PREM undergrad and masters students from North Carolina Central University (NCCU) (center in burgundy) and Cal State LA (on the right in black/gold) who were spending the summer in 2016 doing research projects as part of MRSEC-affiliated REU program. Credit: Kristin Dreyer/Penn State

"This partnership expands the depth and scope of materials research at NCCU, providing NCCU students and faculty with opportunities to work with world-leading faculty and facilities at Penn State to study emerging properties of novel nanoscale systems," said Marvin Wu, NCCU professor of physics and PREM co-principal investigator. "The partnership also leverages Penn State MRSEC resources to prepare NCCU students for STEM graduate study or industrial careers by giving them first-hand experience with the scale of research and academic demands at a major research institution, and providing academic support, career guidance, and professional development activities."

The PREM partnership with FIU is new, but is the result of a relationship between FIU around Penn State's 2D Crystal Consortium Materials Innovation Platform (2DCC-MIP) that goes back five years. The 2DCC is a national user facility, supported by NSF, that is focused on advancing the synthesis of 2D layered chalcogenides for next generation electronics and quantum technologies. It includes state-of-the-art equipment for bulk crystal growth, thin film deposition, and in situ characterization as well as expertise in theory and simulation which was of interest to FIU.

"We initially got connected with Daniela Radu, the primary investigator at FIU," said Joan Redwing, director of the 2DCC and synthesis lead, and professor of materials science and engineering and electrical engineering. "Once they learned about the 2DCC and the facilities that we have, they submitted a proposal to become users of the 2DCC. Over the

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years, we've written a couple of joint grant proposals with them, including one funded by NASA's Minority University Research and Education Project (MUREP) Institutional Research Opportunity, so we already have an existing collaboration with them."

Radu said that the benefits her students see from the PREM program are many.

"The center aims to foster student training and mentoring in quantum science, with focus on inclusion of underrepresented minorities and women," said Radu, who is an associate professor of mechanical and materials engineering at FIU. "The participating students will have the opportunity to engage in the collaborative research of the NSF PREM IMPAQT center, benefiting from the student exchange program and various professional development activities that we planned in tandem with 2DCC. " ■

More information on the Penn State PREM programs can be found at https://www.mrsec.psu.edu/mrsec-research.

Participants in the Partnership for Research and Education in Materials (PREM) program in 2019 walk students through a science demonstration at the Penn State Science-U Make It Matter camp. The PREM students left to right against the wall are Michael Cruse from North Carolina Central University, David Reyes-Ramirez from California State Los Angeles and Brett Green from Penn State Credit: Penn State

PENN STATE CENTER UNVEILS INNOVATIVE NEW K-12 MATERIALS SCIENCE CONTENT

By Jamie Oberdick

THE PENN STATE Center for Nanoscale Science recently went on a mission: To create new online content for K-12 students to learn about materials science and the impact it has on everyday lives.

The center recently published five new DIY-at-home activities on its Mission: Materials Science website. Such work fits the center's overall mission as a National Science Foundation (NSF) Materials Research Science and Engineering Center (MRSEC), one of 19 in the United States. MRSECs support collaborative, interdisciplinary research, and educational efforts, including K-12 outreach activities such as "Mission: Materials Science."

MISSION: MATERIALS SCIENCE

The new activities were directly inspired by the research interests of contributing scientists, but educational needs that arose during the COVID-19 pandemic and a desire to map the mission site's activities closer to the Next Generation Science Standards (NGSS) created a timely opportunity to broaden the site's initial audience. The NGSS was created by a national collaboration of educational experts to improve science education for all students, and many states have adopted it for their own standards. By including NGSS references, the site becomes a resource for educators as well as kids.

"During the pandemic, when in-person events with kids were not possible, the center's Outreach Team Leader Ciera Wentworth decided to embrace the challenge of mapping and updating the site's existing activities to the NGSS so that the content would be more easily accessible to classroom teachers," said Kristin Dreyer, program director for education and outreach for the Center. "Her efforts included tapping NGSS and educational research experts to learn more about the standards, how to use them and why they matter."

Compared to the original eight activities, most of which were repurposed from prior outreach development efforts, the updated content was inspired and developed from start to finish by current researchers every step of the way. Two of the five new K-12 "DIY-at-home" activities were created by Penn State graduate students and faculty; one by researchers at North Carolina Central University, the center's partner in the NSF's Partnership for Research and Education in Materials (PREM) program; and two by students and a staff member at the University of Pennsylvania's MRSEC.

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Mikayla Mathis, a student at Freire High School in Philadelphia, shooting a video in studio. Credit: WPSU. All Rights Reserved.

All of these included 10 new videos produced by Kristian Berg, senior producer at WPSU Penn State.

In addition, the center worked with a long-standing partner, the Franklin Institute (TFI) in Philadelphia, and another new local science museum partner, Discovery Space of Pennsylvania. TFI's relationship with the center began in 2001 and includes the past development of six sets of hands-on, interactive, materials-related tabletop activities. Eventually, this same interactive approach was applied to the virtual platform of Mission: Materials Science, but engaging local audiences via in-person programming remains an important priority.

"The Franklin Institute has been collaborating with Penn State's Center for Nanoscale Science for over 20 years, demonstrating how university researchers and science museums can bring together cutting-edge research and expertise in STEM learning to engage public audiences of all ages," said Jayatri Das, chief bioscientist at TFI. "For Mission: Materials Science, our team brought this expertise to put materials science into the hands of kids — guiding development of DIY activities that empower kids to explore, test, and discover surprising properties of everyday materials at home and make connections to real-world innovation at Penn State and other universities."

TFI played a key role in facilitating the new Mission: Materials Science digital-content development approach by providing informal science education training to researchers via its Science Engagement Institute program, a new customized online seminar and workshop series which teaches researchers how to create, present, and evaluate engaging and effective outreach activities for youth.

"Many children turn away from STEM because they do not see themselves as scientists. Therefore, it is important for students of all ages to see and interact with actual scientists," said Brooke Bernardoni, science instructor, Discovery Space

"Along with the great activities, I love that Mission: Materials Science introduces kids to real people doing science," Das said. "There are lots of videos on the site that help kids do the activities and learn about materials research, and none of the people featured are actors. Kids get to see other kids from the Franklin Institute's youth programs, along with students, faculty, and staff from Penn State and other universities.

"It's a wonderfully diverse group of people that helps kids see the human face of science and envision a place for themselves in the field." ■

GETTING A HEAD START ON A MATERIALS RESEARCH CAREER

Materials Research Institute gives undergraduate student workers an opportunity to gain valuable experience

By Jamie Oberdick

FACED WITH a growing workload in its research labs, the Materials Research Institute (MRI) met the challenge by offering Penn State students an opportunity that most materials science and engineering undergraduates normally never receive.

Within MRI's state-of-the-art lab facilities in University Park's Millennium Science Complex, a wide variety of research work is carried out daily. Along with being the center of materials research at Penn State, MRI also offers a variety of user services to both Penn State and external researchers. This includes sample fabrication and characterization by MRI's Nanofabrication Laboratory and Materials Characterization Laboratory (MCL) for hundreds of industry, government and university users. In addition, there are outreach activities such as providing research support to primarily undergraduate institutions through the National Science Foundation Materials Research Science and Engineering Centers' Materials Research Facilities Network (MRFN).

The combination of growing utilization of the MCL by the Penn State community coupled with an interest in expanding outreach activities created a workload that required some outside-the-box thinking to keep up with demand.

"We kicked around a bunch of ideas to address these opportunities, and one of them was what if we took the time to invest in hiring some bright Penn State undergraduate students so that they could help the lab achieve some of our goals over the summer," said Josh Stapleton, MCL Director and MRI staff scientist.

Connor Mosebey (center) loads a materials sample into a UV-Vis spectrometer while Materials Research Institute researchers Nichole Wonderling (left) and Josh Stapleton (right) observe his work in the Millennium Science Complex on the University Park campus. Credit: Penn State MRI

Some of the students were trained to become proficient in basic TEM operations. TEM refers to transmission electron microscopes, a key tool in materials characterization where a thin specimen, ideally less than 100 nanometers, is exposed to an energy electron beam for high-resolution imaging.

"An entry-level TEM operator can do things such as load and unload samples, carry out basic imaging, and do ►►►

basic elemental mapping," Stapleton said. "While this may sound simple, it's a complicated process that requires time to master. We provided the students with ample time to learn the technique and become proficient. It's rare to have undergraduate students perform this sort of high-level work in part due to the investments that is needed for them to become independent."

According to Stapleton, with the workload ever increasing, the need for an innovative solution was clear, so they hired a group of students to work in MCL over the summer. These students were then teamed with MRI staff scientists to receive a level of training that normally only graduate students receive.

One student, Bevan Harbinson, a junior majoring in materials science and engineering, worked with Trevor Clark, MCL staff scientist, to become an independent TEM operator. His primary task was to support one of the 2021 MRFN researchers, Kate Plass at Franklin and Marshall College in Lancaster.

"There is a lot of underutilized time on the TEM schedules during the off hours and Kate wanted to use it remotely but needed someone to load samples and support the students," Clark said.

To fill this need, Harbinson was trained by Clark on a transmission electron microscope. This training and experience enabled him to support remote operation of the TEM by exchanging samples, working out technical issues, and helping the remote users get quality images and data from their samples.

"I have spent close to 200 hours on the electron microscopes this summer, more than many materials science graduate students get during their entire time at the University, so I have become quite proficient on many of the electron microscopes here at Penn State," Harbinson said.

Another student is Connor Mosebey, junior majoring in chemical engineering, who was trained in the X-ray scattering lab by Nichole Wonderling, X-ray scattering manager with MRI, and Gino Tambourine, lab assistant with MRI.

"Connor is a bright young man and he learned operation of the X-ray diffraction and other instruments quite quickly," Wonderling said. "Within just a few weeks Connor was able to provide meaningful support to our staff."

Mosebey's role as an undergraduate research assistant in the MCL included work in the X-ray lab, particle sizing, and ultraviolet/visible spectroscopy.

"Being familiarized with all these techniques as an undergrad has been an invaluable experience that will help me throughout my future career, wherever that may take me," Mosebey said.

Anthony Diaz-Huemme, a junior in materials science and engineering, worked with Jeff Shallenberger, MCL associate director and Stapleton. Diaz-Huemme received a range of experience during his two summer months with MRI. He performed sample prep methods for triple argon ion beam polishing system and learned how to operate surface characterization equipment to study surface topographic features of a series of treated samples for an external partner of MRI and pitched in on a variety of other small characterization projects.

His summer work was Diaz-Huemme's first job in his chosen field, something he found remarkable given he is an undergraduate student.

"I have had the benefit of working hands-on with samples and machines that many of my fellow students only dream of seeing," Diaz-Huemme said. ■

Credit: Pixabay

Penn State awarded $3.4 million contract to target plastic waste

PENN STATE HAS been awarded a $3.4 million contract from the REMADE Institute, a public-private partnership established by the United States Department of Energy, to fund research targeting the inefficient methods currently used to process and upcycle mixed plastic waste. The project is one of 22 projects recently funded by REMADE. The project will receive $1.7 million in federal funds with an additional $1.7 million in cost-share by the project partners.

A global analysis of all mass-produced plastics found that a total of 8.3 billion metric tons of virgin plastics is estimated to be generated worldwide to date. As of 2015, 79% of plastic waste, which contains numerous hazardous chemicals, has been left to accumulate in landfills or natural environments with approximately 12% incinerated and only 9% recycled.

Upcycling is a process of recycling where the resulting product is of a higher value than the original item that was discarded. The research team led by Hilal Ezgi Toraman, assistant professor of energy engineering and chemical engineering, is developing a flexible, two-stage chemical recycling process that decomposes multiple types of plastic and then converts to valuable chemicals that can be used to create new products.

Through the funding, "Chemical Recycling of Mixed PET/Polyolefin Streams Through Sequential Pyrolysis and Catalytic Upgrading," the interdisciplinary team will simultaneously assess the financial and environmentally viability of bringing the proposed process from the lab to the industrial scale based on integrated techno-economic analysis and life cycle assessment tools.

The first step to developing the new upcycling process hinges on a better mechanistic understanding of how dynamic plastic waste mixtures decompose and interact in chemical recycling processes. Built on Toraman's past work, decomposition of plastic waste will be instigated via high temperatures in micro-pyrolysis setups. The study focuses on two of the most common plastics, polypropylene (PP), and polyethylene terephthalate (PET) which are found in multilayered packaging, carpeting residue, and films.

In the proposed two-stage process, the second step is to convert the PET, PP mixture pyrolysis products using low-cost, stable catalysts to valuable chemicals such as benzene, toluene, xylene, and olefins. ■

Materials Research Institute announces 2022 seed grant recipients

Grants to help fund variety of interdisciplinary high-impact, materials-focused research

THE PENN STATE Materials Research Institute (MRI) has announced the 2022 recipients of seed grants that will enable University faculty to establish new collaborations with partners outside their own units for the exploration of transformative ideas for high-impact materials science and engineering. There are four research themes for the seed grants, with 18 grants awarded by MRI in partnership with Penn State's Applied Research Laboratory, College of Medicine, Huck Institutes of the Life Sciences, and the Pennsylvania Recycling Markets Center in Harrisburg, Pennsylvania.

"We're working on some strategic areas and looking to extend our support to different types of teams across the University," said Clive Randall, director of MRI and distinguished professor of materials science and engineering. "In some cases, like the regenerative medicine area under the convergence category, this was to start initial conversations. We anticipate much more growth in this area and going forward is a strategic priority for the University. But we were very happy with all the proposals, including the ones we didn't fund, so much so comments were supplied to those proposals that we did not fund for their future reference and fit for other seed grant programs that are upcoming."

The seed grants were awarded to tenured/tenure track and fixed-term research faculty who hold an appointment of half-time or more at any Penn State location, including staff researchers at the Applied Research Lab and Hershey Medical Center. The time frame for grants is 18 months from the date of award, which started in the first quarter of 2022.

The seed grant research themes include Sustainable Materials; Quantum Device Chip Packaging and Quantum Systems; Convergent Research at the Intersection of Materials – Life – Health – Environment; Integrated Projects in Data Science; Advanced Characterization, and Materials Processing; and MRI-ARL Partnership.

Mike Hickner, associate director of MRI, co-director of CIMP-3D, and professor of materials science and engineering concludes, "Seed grants have been an ongoing priority for MRI and this new round of grants demonstrates our commitment to diverse teams attacking important problems. We are excited to see what new programs can be built upon these seeds and we look forward to fruitful collaborations across the wider Penn State." ■

research SNAPSHOTS

Research Snapshots are brief summaries of significant materials-related breakthroughs by Penn State researchers.

Ally Bythell, a 2021 Penn State graduate who earned her bachelor of science in biomedical engineering and mechanical engineering, crocheted the world's first example of yarn made from Squitex fiber. Credit: Ally Bythell/Penn State

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Full articles on all snapshots can be read at **mri.psu.edu/news**

From waste to wear: How squid may be key to material revolution

By Ashley J. WennersHerron

WITH ELONGATED BODIES, large eyes, and a combination of arms and tentacles, squid appear alien. In reality, they are one of the oldest classes of animals on the planet. Squid evolved during the Jurassic period and now appear in every ocean around the world. They are ubiquitous across literature and cuisine alike, popping up in stories and on plates since at least the fourth century B.C., when Aristotle first described the beasts in "The History of Animals."

Now, nearly two and a half millennia later, squid may be the answer to a modern dilemma — plastic pollution. Melik Demirel, Penn State Lloyd and Dorothy Huck Chair Professor in Biomimetic Materials and professor of engineering science and mechanics, leads a research team investigating how to mimic nature in an effort to mitigate damage caused by humans.

Demirel launched his research project a decade ago, focusing on the sharp, circular teeth found in the suction cups of squid tentacles. These ring teeth help squid hold onto their prey. They are durable, flexible structures that can heal themselves without losing strength or function. The teeth's proteins are responsible for this evolutionary benefit, and his team introduced the proteins to E. coli bacteria, which can perpetually reproduce the proteins in significantly greater quantities.

"The squid ring teeth proteins are similar to silk, like that made by spiders, but they evolved in water," Demirel said, noting that spider silk tends to shrink in water.

The researchers ferment the proteins using sugar, water, and oxygen. The resulting mash is dried into a powder, which is processed through a wet spinner, which sprays out strands of water containing the powder. The wet spinner spins, twisting the strands into a fiber the researchers augment with either acrylic or cellulose to enhance their recyclability, according to Demirel. The result is a composite fiber Demirel calls Squitex.

The proteins are made of amino acids that repel each other and slip apart at the atomic scale, producing unusual tangles of biological material — which, in turn, can be manipulated into flexible, biodegradable fiber strong enough to lift 3,000 times its own weight. In 2020, Demirel co-authored a Nature Materials paper on the proteins.

The process is currently expensive and slow, according to Demirel, but the potential is limitless.

"This has demonstrated that we can make chemicals from a bio-based economy, and the applications are immense," Demirel said. "And, of course, the process is circular: The squid protein-based materials can be made from carbon dioxide-absorbing organisms, so they are not only biodegradable, but they help mitigate carbon emissions. We're going step by step, but we want to accelerate the process. To go from genes to yarn in 10 years, we expect the next 10 years to result in even greater steps forward." ■

research SNAPSHOTS

Salvaging rare earth elements from electronic waste

Amir Sheikhi, Penn State assistant professor of chemical engineering, found a new process to separate and recycle rare earth elements using plant cellulose, an inexpensive renewable resource found in paper, cotton, and pulp, like the paper towel shown here. The vial contains the nanoparticles that are used to separate rare earth elements from old computers and circuit boards. Credit: Kate Myers/Penn State

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Solving the 'big problems' via algorithms enhanced by 2D materials

By Jamie Oberdick

IMPORTANT OPTIMIZATION ALGORITHMS that are designed to solve large-scale problems such as airline schedules and supply chain logistics may soon get a boost from 2D materials that will enable the algorithms to better solve the problems and use less energy, according to Penn State researchers.

These large-scale issues are known as combinatorial optimization problems, the term for a set of problems that are so complex that finding the best solution using an exhaustive search is sometimes unfeasible. Therefore, algorithms are valuable tools in solving these problems by finding the best possible solution.

"These are problems that we face in our everyday life, such as scheduling of transportation or supply chain logistics, and you need to really optimize the best way of doing it correctly," said Saptarshi Das, associate professor of engineering science and mechanics and primary investigator for the study that was recently published in Advanced Materials. "One famous example is the Traveling Salesman Problem, where a salesman has to go from city A to city B to city C to city D, but he has to find the optimal route where he can visit each city exactly once in the shortest time and return home."

The key is overcoming a bottleneck that forms during the transfer of data between memory and the computational unit that happens when a computer tries to solve a combinatorial optimization problem, known as a von Neumann bottleneck.

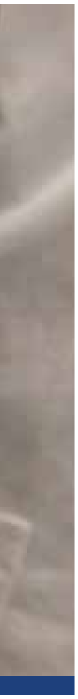
"With all the scheduling and logistic problems, you are dealing with a lot of data, and then you have a lot of computation, and every time you have to essentially shuttle this huge amount of data to the computing, do the computation, bring it back and do it again," Das said. "These processes consume a lot of energy, this shuttling of the data between your storage and your computation."

The researchers propose a solution that combines an optimization algorithm known as simulated annealing with a technique known as in-memory computing. The researchers propose using a simulated annealing algorithm to find the ground state of an Ising spin glass system. To do this, they need to do high-end computational operations, and to carry out these computations, they used 2D materials.

"In order to implement simulated annealing, we perform certain computational operations in hardware," said Amritanand Sebastian, doctoral student in engineering science and mechanics and

By Mariah Chuprinski

MANUFACTURERS RELY ON rare earth elements, like neodymium, to create strong magnets used in motors for electronics including hybrid cars, aircraft generators, loudspeakers, hard drives, and in-ear headphones. But mineral deposits containing neodymium are hard to reach and are found in just a few places on Earth.



With rising need for neodymium from several industries, attention has turned to recycling the elements found in old computers and printed circuit boards, otherwise known as electronic waste, to meet demand. But separating the valuable elements from other minerals and components found in e-waste proves to be a challenge.

In a recent paper in the Chemical Engineering Journal, Amir Sheikhi, assistant professor of chemical engineering and biomedical engineering, at Penn State, details a new nanotechnology to separate neodymium using plant cellulose, which is found in paper, cotton, and pulp.

In the process, hairy cellulose nanocrystals, nanoparticles derived from cellulose fibrils, bind selectively to neodymium ions, separating them from other ions, such as iron, calcium, and sodium, according to Sheikhi. The nanoparticles are known as "hairy" due to cellulose chains attached to their two ends, which perform critical chemical functions.

To do this, the researchers negatively charged the hairy layers of the nanoparticles in order to attract and bind with the positively charged neodymium ions, resulting in particle aggregation into larger pieces that can then be effectively recycled and reused.

Current rare earth element recycling processes are environmentally detrimental, according to Sheikhi. They often use highly acidic conditions to extract the elements in chemical reactions. Sheikhi's process is environmentally friendly due to its use of cellulose, which is an inexpensive renewable resource. The traditional mining process is dangerous and expensive, with harmful environmental impacts from open-pit mining.

"Using cellulose as the main agent is a sustainable, cost-effective, clean solution," Sheikhi said. "Using this process, the United States will be able to compete with other giants like China to recover rare earth materials and independently produce them."

China is the leading exporter of neodymium, according to Sheikhi, exporting more than 70% of the world's supply of the material.

In addition to e-waste, rare earth elements like neodymium can be extracted from industrial wastewater, mining tails, and permanent magnets that are no longer in use. In the future, Sheikhi said he hopes the cellulose-based adsorption process can be applied to those sources as well.

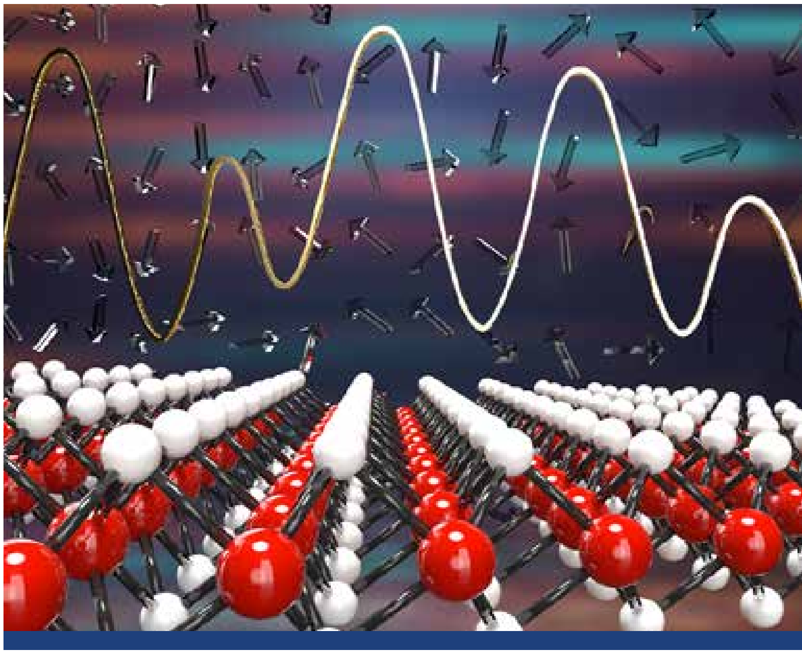
"This contribution to rare earth recycling will have a strategic and economically-viable impact on several industries," Sheikhi said. "The more neodymium we recycle, the more we can manufacture electric and hybrid vehicles and wind turbines, leading to less strain on the environment." ■

co-author of the study. "The hardware is implemented using 2D material-based transistors. In addition to performing computations, these transistors can also store information. We make use of this in-memory computation capability in order to perform simulated annealing in an efficient manner."

Using 2D materials for this purpose makes sense, according to Das, as 2D materials in general hold potential for future electronics and possibly an alternative to silicon technology.

"We all know that silicon technology is aging, even if it is still a very robust technology that is very difficult to compete with," Das said. "But we also know that 20 years down the line, we may have to augment the silicon technology, if not completely replace it. The unique functionalities of 2D materials that work so well for our purposes in this study make it one of the prime candidates for replacing silicon at some point."

Along with Das and Sebastian, an additional author of the study is Sarbashis Das, doctoral candidate in electrical engineering. The Department of Defense and National Science Foundation supported this research. ■



Representation of simulated annealing using a 2D material (molybdenum disulfide) for the optimization of Ising spin system, which is a magnetic system characterized by the randomness in spin orientations. Credit: Jennifer M. McCann/Penn State

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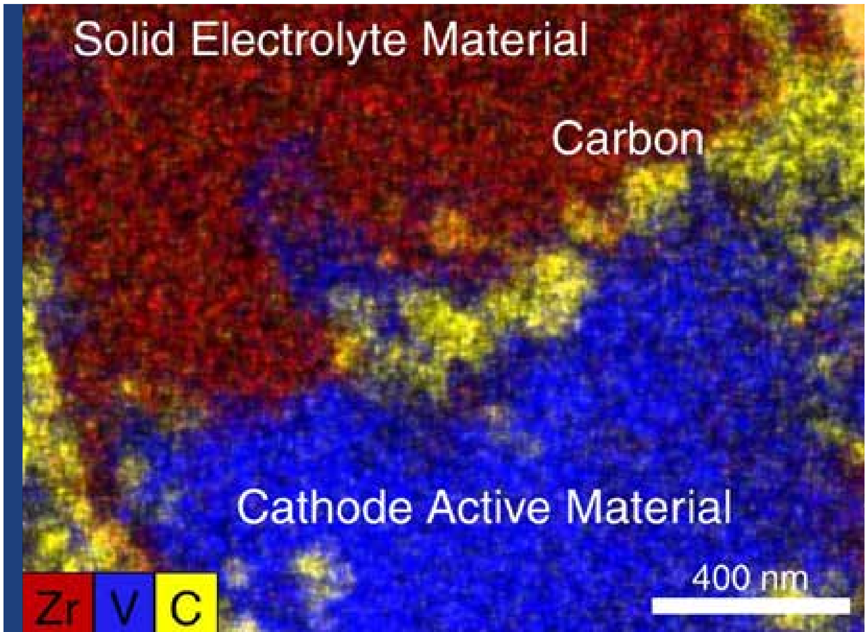

Cold sintering allows for the fabrication of composites with three components; the active material, the solid electrolyte, and the carbon fiber. This unique microstructure provides both the ionic and electronic pathways necessary to drive the redox reaction in the electrode in a solid-state battery. Credit: Zane Grady/The Randall Group

Cold-sintering may open door to improved solid-state battery production

By Jamie Oberdick

COMPARED TO THEIR traditional battery counterparts, solid-state batteries have higher energy potential and are safer, making them key to advancing electric vehicle development and use. Penn State researchers have proposed an improved method of solid-state battery production that enables multi-material integration for better batteries — cold sintering.

Traditional batteries have a liquid electrolyte, which enables the ions to move between the cathode and the anode, the battery's two electrodes. Solid-state batteries have a thin electrolyte made of a solid material.

"Solid-state batteries have a lot of advantages from a safety perspective in that they don't catch on fire, because they're a lot more stable owing to their stronger bonding," said Zane Grady, doctoral student in materials science and lead author of the study that was published in ACS Applied Materials & Interfaces. "Because of that stronger bonding, they are also more mechanically robust. This prevents fire-causing short circuits, but also in theory it enables solid-state batteries to have higher energy density. They have an order of magnitude increase in performance relative to the batteries that we have now, which are reaching their limit."

One of the larger issues for solid-state batteries making the leap from laboratory to the market is the great challenges inherent in their production. According to the researchers, cold sintering may offer a solution. Cold sintering is a revolutionary process that enables sintering of ceramics at a much lower temperature than traditional methods, therefore using much less energy and enabling potential new material combinations. It was developed at Penn State by the research team led by Clive Randall, director of the Materials Research Institute, distinguished professor of materials science and engineering, and co-author of the study.

In a prior study, the research team demonstrated how cold sintering can be employed at temperatures below 300 degrees Fahrenheit (150 degrees Celsius) to fabricate multilayered, solid-state lithium-ion batteries. They relied on conductive salts to obtain suitable electrochemical properties, which undercut some of the conductive and safety advantages of solid-state batteries. Then, the team demonstrated that a solid electrolyte comprised of sodium zirconium silicate phosphate, often colloquially referred to as the NASICON solid electrolyte, could be cold sintered at a slightly higher temperature, 707 degrees Fahrenheit (375 degrees Celsius), by replacing the liquid transient solvent with a more reactive, solid sodium hydroxide transient solvent. This resulted in a highly conductive ceramic solid electrolyte without the use of any additional conductive salts.

For this current study, the team demonstrated a novel route toward the fabrication of mixed conducting electrodes for solid-state batteries. The team took a NASICON cathode ceramic powder that is densified into a ceramic composite pellet with a transient solvent to help it densify, and used a carver press to apply necessary pressure to the powder. The pressure is applied and heated for three hours at 707 degrees Fahrenheit (375 degrees Celsius).

The U.S. Department of Energy and the U.S. Department of Defense supported this research ■.

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Full articles on all snapshots can be read at **mri.psu.edu/news**

Study challenges standard ideas about piezoelectricity in ferroelectric crystals

By Jamie Oberdick

FOR YEARS, RESEARCHERS believed that the smaller the domain size in a ferroelectric crystal, the greater the piezoelectric properties of the material. However, recent findings by Penn State researchers have raised questions about this standard rule.

Ferroelectric materials possess spontaneous electric dipole moments that can be reversibly flipped by applying an electric field. Domains are areas in the ferroelectric crystal that have the dipole moments aligned in the same direction. Piezoelectricity is a material property where the crystal generates electrical charge under an applied mechanical force. This capability enables piezoelectrics to be used in electronics, sensors, and actuators.

"So many devices in our daily life utilize the ability of a material to convert electrical signals to mechanical signals and vice versa," said Bo Wang, postdoctoral scholar in materials science and engineering. "In most of these applications, the piezoelectric material plays a key role. And the most advanced piezoelectric materials are the ferroelectric materials."

At a microscopic scale, ferroelectric materials consist of many domains, and these domains range in size from a few nanometers to as much as millimeters. Each domain consists of uniform or nearly uniform distribution of dipole moments, which occur when there is a separation of charge. The regions between adjacent domains are known as domain walls.

"There is a general belief in the community that the smaller the domain size or higher the domain wall density, the larger the piezoelectric coefficient," Wang said.

However, the recent work by Wang and his co-workers, published in Advanced Materials, challenges this conventional wisdom.

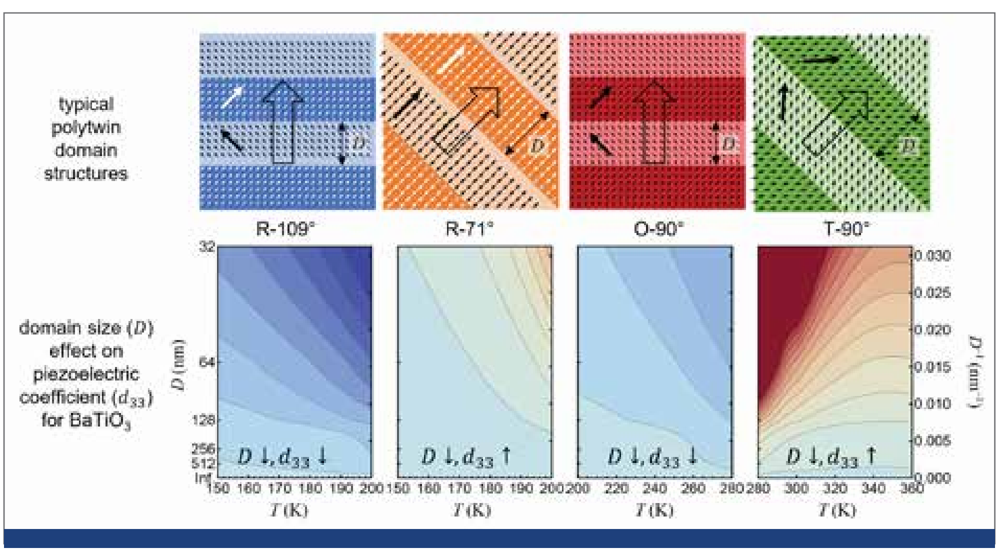
The researchers found that the idea that smaller domains lead to higher piezoelectricity is based on very limited existing data without a solid theoretical foundation.

"Based on this conventional wisdom, many in the research community have tried to find ways to make all these domains smaller to enhance the piezoelectricity, and often when they see some improvement in the piezoelectric performance, one of the first things that comes to mind is maybe due to the smaller domains," said Long-Qing Chen, Hamer Professor of Materials Science and Engineering, professor of engineering science and mechanics, and professor of mathematics at Penn State. "Our work provides a theoretical foundation for correlating the piezoelectricity to crystal symmetry, crystal orientation, and domain configuration."

In that paper, they referred to findings by other researchers that an AC electric field can improve the piezoelectric response of the crystal by 20% to 40% compared with the crystal treated by a DC electric field. But the team discovered that inside the crystal during AC switching cycles, the domain sizes actually got bigger, not smaller as would be expected. According to Wang, this new understanding of the relationship between ferroelectric crystal domain size and piezoelectricity can provide guidance to improve piezoelectric performance of materials.

Along with Wang and Chen, the other author on the study was Fei Li, a previous postdoctoral researcher in materials science and engineering at Penn State and now a full professor at Xi'an Jiaotong University in China.

The National Science Foundation supported this research. ■



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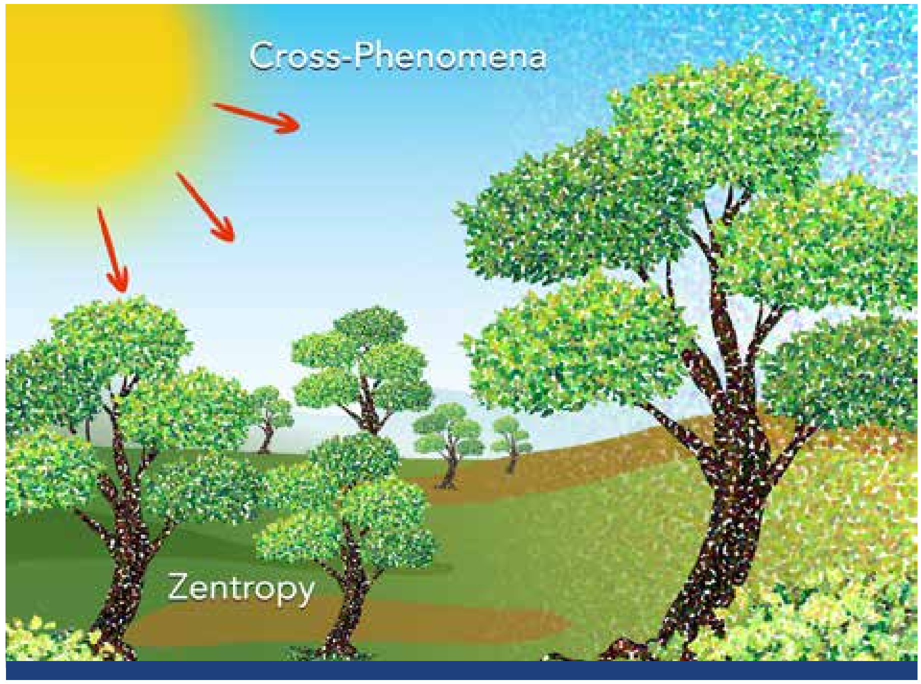
Schematics of domain structures of barium titanate single crystals (upper panel) and the corresponding piezoelectric coefficient as a function of the domain size and temperature (lower panel), which are calculated by phase-field simulations.
Credit: Chen Research Group

research SNAPSHOTS



Entropy is the measure of the disorder in a system that occurs over a period of time with no energy put into restoring the order. Zentropy integrates entropy at multiscale levels. Credit: Elizabeth Floresgomez Murray

The zen of zentropy
novel theory of entropy may solve materials design issue

By Jamie Oberdick

A CHALLENGE IN MATERIALS design is that in both natural and manmade materials, volume sometimes decreases, or increases, with increasing temperature. While there are mechanical explanations for this phenomenon for some specific materials, a general understanding of why this sometimes happens remains lacking.

However, a team of Penn State researchers has come up with a theory to explain and then predict it: Zentropy.

Zentropy is a play on entropy. Zentropy theory notes that the thermodynamic relationship of thermal expansion is equal to the negative derivative of entropy with respect to pressure, i.e., the entropy of most material systems decreases with an increase in pressure. This enables Zentropy theory to be able to predict the change of volume as a function of temperature at a multiscale level, meaning the different scales within a system. Every state of matter has its own entropy, and different parts of a system have their own entropy.

The authors of the study, published in the Journal of Phase Equilibria and Diffusion, believe that Zentropy may be able to predict anomalies of other physical properties of phases beyond volume. Macroscopic functionalities of materials stem from assemblies of microscopic states (microstates) at all scales at and below the scale of the macroscopic state of investigation (macrostate). These functionalities are challenging to predict because only one or a few microstates can be considered in a typical computational approach such as the predictive ab initio calculations, which help determine the fundamental properties of materials.

“This challenge becomes acute in materials with multiple phase transitions, which are processes that convert matter from one state to another, such as vaporization of a liquid,” Liu said. “This is often where the most transformative functionalities exist, such as superconductivity and giant electromechanical response.”

Zentropy theory “stacks” these different scales into an entropy theory that encompasses the different elements of an entire system, presenting a nested formula for the entropy of complex multiscale systems, according to Liu.

"You have these different scales and you can stack them up with Zentropy theory,” Liu said. “For example, atoms as a vibrational property, that's low scale, then you have electronic interaction, that even lower scale. So now how do you stack them together to cover the entire system? So that is what the Zentropy equation is about, stacking them together. It creates a partition function that is the sum of all the entropy scales.”

Zentropy has potential to change the way materials are designed, especially those that are part of systems that are exposed to higher temperatures. These temperatures, given thermal expansion, could cause issues if the materials expand.

The work was supported by the National Science Foundation, the Department of Energy, and the Department of Defense. ■

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Michael Janik (left), Penn State professor of chemical engineering, and Robert Rioux, the Penn State Friedrich G. Helfferich Professor of Chemical Engineering, published a Nature Chemistry paper wherein which they tested efficient, customizable catalytic reactions that cut down on unneeded competitive reactions and isolated a successful, predictable one. Credit: Kelby Hochreither/Penn State

Precise control of atomic arrangement may mean less waste in producing plastic

By Mariah Chuprinski

IN THE LAST 20 years, there have been efforts to reduce fossil fuel use in plastics manufacturing, and, according to Penn State researchers, efficient, customizable catalytic reactions — where two metals are combined using a catalyst, or molecule that remains unchanged during a reaction — are an attractive alternative.

Researchers have found a way to make catalytic reactions less wasteful and more cost effective by controlling the placement of each atom on the catalyst surface. Controlling or customizing the catalysts cuts down on unneeded competitive reactions and isolates a successful, predictable reaction. These results were published in Nature Chemistry.

"By isolating an active metal in an inert host, and precisely controlling the exact ratio of the metals, we can get a targeted pattern of the two metal atoms," said Michael Janik, Penn State professor of chemical engineering and co-principal investigator for the study.

Researchers used palladium, which served as the active catalyst component, and zinc, the inert host, to form an intermetallic, a compound with two or more types of metal atoms arranged in a repeating pattern.

The researchers, led by Janik and co-principal investigator Robert Rioux, the Penn State Friedrich G. Helfferich Professor of Chemical Engineering, tested different amounts of zinc and palladium and found that different ratios of zinc-to-palladium had widely different catalytic reactivity.

The researchers tuned the ratio of palladium to zinc to form surfaces that contained only isolated palladium monomers and trimers, or clusters of three adjacent atoms. They demonstrated that both palladium monomers and trimers could hydrogenate —or add hydrogen gas to — acetylene, and thus create ethylene, a gas needed to process plastics.

But in the process, palladium trimers also catalyzed an ethylene hydrogenation reaction, an undesired consequence, which ruled out using trimers. Isolated palladium monomers surrounded by zinc atoms, however, were an effective configuration for selectively hydrogenating acetylene.

Because of their work on this paper, Janik, Rioux, and their collaborators received a $1.2 million grant in 2019 from the U.S. Department of Energy with the goal to extend the science into new applications.

"We will use computational modeling and machine learning to predict designs of other intermetallics that will arrange certain numbers of metal atoms in unique configurations," Janik said. "We are now trying to find other combinations of two metals that allow us to control the arrangement of the two metal atoms."

Janik, Rioux, and collaborators at Penn State and Carnegie Mellon University are now using data science approaches to discover other intermetallic catalysts with precise and tunable reaction sites. Working with Zachary Ulissi, associate professor of chemical engineering at CMU, they coded a publicly available web application, known as Nuclearity Zoo, which calculates the arrangement and shape of any combination of active and inactive metals and lists all the potential atomic arrangements of them. The app uses graph theory approaches to categorize active site shapes and sizes.

The research group is now using the app and data science approaches to computationally predict active and selective catalysts for a number of industrially important reactions.

Support for this work was provided by National Science Foundation and the U.S. Department of Energy. ■

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Full articles on all snapshots can be read at **mri.psu.edu/news**

The ‘one mat
community’ a

PENN STATE HAS built a community and culture of interdisciplinary research that is the envy of its peers. So much so, a research team from the University of California, Riverside published an article in The Journal of Higher Education in December 2019 that singled Penn State out as a unique example of a university that found great success in interdisciplinary research.

This success is due to Penn State building a structure that enables research to happen across disciplines, campuses, departments, and institutes. Penn State’s seven interdisciplinary research institutes, of which the Materials Research Institute (MRI) is one, is the foundation of this structure.

This structure has enabled MRI to build collaborations in materials research that connect researchers in a way that has led to many triumphs. This success is reflected in Penn State’s number one ranking in materials science and number two ranking in materials engineering, according to the latest National Science Foundation rankings of Higher Education Research and Development (HERD) research expenditures, released in January 2022.

“Penn State has a vision for a ‘one university’ type model, for example, last year we announced the One Penn State 2025 initiative which is about creating this seamless, interdisciplinary learning experience that stretches across the entire system,” said Clive Randall, distinguished professor of materials science and engineering and director of the Materials Research Institute. “This is something we’ve already been doing on the research side for a while now, and we in MRI have worked with others at the University to create a ‘One Materials Community.’”

erials at Penn State

This "One Materials Community" at Penn State produces research that not only enables the University's materials research to be highly regarded by peers but also has an impact. Given each of us is surrounded by them, materials are part of our lives in many different ways. This includes the visible and obvious, such as new building materials in the rooms we are sitting in, and the not-so-obvious, such as 2D materials that are inside our electronics.

MRI's research ranges from clean energy to structural materials to healthcare to electronics to 5G to Industry 4.0. This impactful research combines new, innovative approaches in materials research with the physical and life sciences, engineering, and computation. This requires breaking out of the silos that can inhibit breakthroughs and seeking out partnerships and collaborations with our Penn State colleagues all across Pennsylvania.

In this section of Focus on Materials, we offer just some of the many examples of this impactful research, that includes partnering with our fellow Penn State interdisciplinary institutes, branch campuses, the Applied Research Laboratory, multiple Penn State colleges, and government and industry. The articles that follow include explorations of the possibilities of Industry 4.0, humanitarian projects that put a human face on materials research, solutions for more sustainable supply chains, work in the powder metal industry that provides thousands of jobs to rural northcentral Pennsylvania, how MRI's centralized facilities provide access to equipment for researchers in our branch campuses, and more.

These stories give just a taste of research that is both immense in scale and diverse in scope and is forward-thinking towards a better future for all through materials innovation. ■

Image: An entrance to Pennsylvania State University in University Park, Pennsylvania on June 21, 2018. Credit: Penn State

Penn State's interdisciplinary institutes drive University's research success

PENN STATE'S RESEARCH model includes seven University-wide interdisciplinary institutes to promote collaborative research that answers vital scientific questions and pressing societal needs. This system has worked well for Penn State's research community, with research expenditures reaching more than $993 million for fiscal year 2020-2021.

As one of these seven institutes, the Materials Research Institute (MRI) has contributed greatly to this achievement, helping Penn State's materials science and materials engineering place number one and number two in the nation, respectively. So, what is the "secret sauce" behind this success? The key is regular communication and collaboration among all the institutes.

"It's a continuous dialogue among leadership in the institutes," said Clive Randall, director of the Materials Research Institute. "We typically meet once a week, if not more, to keep each other informed as much as we can. The goal is just awareness. For example, if we're going to pull a seed program together, and we know that there is an opportunity for overlap with a different institute, there's usually a dialogue to share agendas, whether the proposals are good fits, and whether ideas that are not good fits may be good for other opportunities."

MRI partners with members across the entire Penn State research institute system, and just two examples of collaborative partnerships that advance impactful materials research are those MRI has with the Institutes for Energy and the Environment (IEE) and the Huck Institutes of the Life Sciences.

With the IEE, MRI collaborates on work involving materials and energy-related applications. The areas of joint research range from solar cells to energy storage to reuse of waste materials, among many others. IEE Director Tom Richard said that one area where high impact research is happening among the institutes is in building materials, an area that Richard said has great societal impact.

"Better building materials and building energy efficiency is really important; building construction and operations represent roughly a third of the global economy," Richard said. "Most of our electricity is used in buildings, so energy efficiency is really important. The embedded carbon in those building materials also is very important, with concrete and steel the two largest carbon-emitting industrial sectors. Sometimes you want to take carbon out of the material due to environmental and climate change concerns, like using fewer plastics made from fossil carbon. But sometimes you want to put the carbon into the material, using biocarbon from photosynthesis for bioplastics or engineered wood structures that can now be over 20 stories tall. We have great faculty affiliated with both IEE and MRI working in both of those directions."

A perhaps surprising area of collaboration within IEE and MRI is social science. The IEE includes affiliated social scientists, and these social scientists are sometimes involved in IEE/MRI collaborative projects.

Credit: Penn State

"The social sciences offer a critically important dimension of interdisciplinary research that includes thinking about the economics, the policy, and the human behavior behind bringing our research to application," Richard said. "There's incredibly rich and important work to be done in what is sometimes called implementation science. This involves the steps to getting a great idea out of somebody's head, beyond the bench, into commercialization, and then widespread adoption. Much of what drives successful implementation is finding synergies between technology, human behavior, and values."

A lot of Penn State research is carried out in the Millennium Science Complex, where MRI shares office and laboratory facility space with the Huck Institutes of the Life Sciences. This space arrangement is ideal, according to Huck Director Andrew Read, because of all the interesting things happening at the interface between the life sciences and the material sciences.

"Imaging is one example," Read said. "MRI needs to able to see the surfaces of materials, but we need to be able to see inside cells, so there is a lot of overlap. MRI offers a lot of state-of-the-art imaging tools that are perfect for this work. Along with imaging, a lot of life science problems can be addressed by material research techniques, such as using sensors, so we have mutually beneficial interests and plenty of research partnership opportunities."

Read added that another, highly impactful area where MRI and Huck work together is cancer research, especially work done by Deb Kelly, director of the Center for Structural Oncology, Huck Chair in Molecular Biophysics, and professor of biomedical engineering.

"Deb is working to figure out why particular mutations cause cancer," Read said. "What is it about a mutated protein that causes the cancer? And that work is right at the interface between materials and life science because of the imaging processes she needs to use. MRI offers the cutting-edge tools she needs to do this work."

The collaborations that MRI has with Huck, IEE, and the other Penn State research institutes are important, Randall said, because of the simple reason that interdisciplinary research gets more results than one-dimensional siloed research.

"Science is a complicated domain, even within a narrow field, so if you have an idea you need to have access to the right people to give input, even just to decide if it needs more exploration," Randall said. "So just in terms of the nurturing, filtering, and developing ideas, it is good to have more than one part of the University involved. The scientific debate has then expanded."

Randall added, "If more than one part of the University can then invest in something then you start building community. If you can build a community, you build critical mass. If you build critical mass around excellence, you can start to build a reputation with a world-class visibility that demonstrates you are capable of addressing the complex and most pressing of issues." ■

Industry 4.0 will change manufacturing. But what about its impact on society?

INDUSTRY 4.0 IS a growing buzzword in both the enterprise and higher education worlds. While there are certainly benefits for enterprise with Industry 4.0, there are also potential benefits beyond industry and for society in general. And the Materials Research Institute (MRI) is exploring both possibilities.

WHAT IS INDUSTRY 4.0?

For those who are not familiar, Industry 4.0 is best described as a combination of traditional industry practices and cutting-edge digital technology such as the Internet of Things (IoT), cloud data storage, and artificial intelligence (AI)/machine learning. The goal of Industry 4.0 is to improve the economy, especially manufacturing, by developing more efficient processes and practices through intelligent automation at scale.

"Industry 4.0 is shorthand for the fourth industrial revolution that's going on right now," said Tim Simpson, "I see two key things that are a sort of digitalization. One is a digital twin, of your process, factory, and product that is a shadow of the real one and captures all the data and information associated with it. Think how Google Maps is a digital twin of your neighborhood, with real-time traffic, restaurant locations, etc."

The other aspect, Simpson said, is how new, improved connectivity will begin to drive Industry 4.0.

"We can use this new 5G and wireless technologies to connect all this digital technology and do new things, have better productivity and efficiency, have more effective distributed manufacturing, all that good stuff," Simpson said.

Simpson is working with MRI on the data gathering aspect of Industry 4.0. For example, his lab does industrial 3D printing of machine parts, and once the part they are 3D printing is finished, they use facilities in MRI's Materials Characterization Lab (MCL) to characterize it.

"The data we gather from the characterization becomes what is called the ground truth," Simpson said "It's the data that you use to train your AI and machine learning algorithms to then figure out if the 3D printing is running properly. So, when MCL people characterize it, we can review the data and say ok, this is the right microstructure, I got the right chemistry, I don't have any pores or defects, and so on.

> "This becomes training data, that allows me to go back and tell the machine that when this sensor goes off or gets above this level, this means something's out of whack and the part I'm printing is going to be bad, so we need to stop the build and correct it."

Along with this, Simpson said that MRI was also key in helping him find partners to work on Industry 4.0 projects at Penn State.

"Clive Randall, the MRI director, is now connecting me with researchers who are working on creating better materials for 5G environments, looking at radio waves and signals and transmission and all those sorts of things," Simpson said. "Clive has been instrumental in making some connections to folks working in that space."

REVITALIZING A COMMUNITY WITH INDUSTRY 4.0

In addition to manufacturing, MRI is also exploring Industry 4.0's potential societal impact and is working with Penn State's New Kensington campus to that end. New Kensington is a classic western Pennsylvania industrial small city, perched on the Allegheny River about 20 miles northeast of Pittsburgh. Like so many of these towns and cities, they are in a process of revitalization.

A major step in this revitalization is the Digital Foundry, located in downtown New Kensington. Penn State New Kensington will open this 15,044-square-feet innovation and manufacturing lab space in spring 2022, which will feature cutting-edge technologies to develop future-ready skills in students and improve outcomes for local business. The lab space will offer training and access to Industry 4.0 software that fuses digital data and the user's equipment into new product development and manufacturing. This facility will be open to regional businesses; K-12 schools; entrepreneurs; University students, faculty, and staff; and workers looking to develop new marketable skills.

“Basically, it started as a virtual makerspace but thanks to the input of consultants sponsored by the RK Mellon Foundation, Sherri McCleary who was at ARCONIC at the time, and the folks at MRI, we pivoted and geared it to help manufacturing meet Industry 4.0,” said Kevin Snider, chancellor of Penn State New Kensington. “There are 5000 small- to mid-sized manufacturers in the area that have no idea industry 4.0 coming. They don't have the time or the capability or the resources to investigate it and how to apply it in their business, but now, they can do all of that in this facility.”

Snider envisions Penn State New Kensington as an Industry 4.0 educational hub as well, providing local students with skills needed to find employment opportunities in an Industry 4.0 world. He sees exciting potential in the combination of helping local students gain new employable skills and assisting local companies with innovation.

"In the Foundry, we will bring companies that will set up in a bay, and in that bay, they'll be able to replicate a line and/or build a digital twin of their machines,” Snider said. “We can help them with whatever pieces of technology that are needed for that particular company's product or problem. We'll do it in a way that allows our students to participate and gain the knowledge and skills they need to succeed.”

Credit: Rebecca Dietrich/Penn State New Kensington

The Foundry is located on Fifth Avenue in New Kensington, which Snider worked with the city to reimagine as the Corridor of Innovation. The Corridor began with Penn State New Kensington's Corner Launchbox effort and early in the process of expanding revitalization to include Industry 4.0 preparation, Snider invited two MRI researchers to see the proposed corridor, Randall and Esther Obonyo, associate professor of engineering design and architectural engineering and director of the Global Building Network. Obonyo's research includes developing materials for resilient low-income housing.

"So, Esther and Clive were walking on the roofs of the buildings, and seeing where some of the residents were living,” Snider said. “And we got done with that tour, Clive turned to me at the end of it and said we're going to help. He has been extremely supportive of some of the work that Esther did with us to look at alternatives for roofing in New Kensington. This partnership made sense because Esther has been involved in a few studies with our faculty members on physical structures and mental health.”

After the Foundry opens, Snider said he looks forward to continuing to work with MRI.

“Esther and Clive were instrumental in helping us think through how we could connect to research at Penn state, and how we should think about and carry out active research that really makes a difference, to consider all the social factors like mental and physical health, skill development, and how it helps the community," Snider said. “Once the Digital Foundry opens up, I really am looking forward to working with Esther, Clive, and others at MRI because the type of change needed to transform the rust belt isn't just about technology.” ■

A more human-focused materials research on display at Penn State

MATERIALS RESEARCH PROVIDES many benefits for society, however, there are those in our world who are often left out of these benefits, due to living in marginalized communities with limited access to resources. There are materials researchers working to remediate this and to develop materials that help these communities solve a variety of issues, in a field that is best described as humanitarian materials science.

One example of the Materials Research Institute's (MRI) efforts in this area includes offering the Materials Matter at the Human Level seed grant program, which last year awarded grants to six teams of researchers to fund materials projects that benefit humankind. Another example is MRI's partnering with the Penn State College of Engineering in the Humanitarian Engineering and Social Entrepreneurship program. Along with these examples, there are MRI-affiliated faculty who are working on their own humanitarian-focused research projects.

To quote from MRI's strategic plan: "In the MRI, we consider all aspects of the impact of our research, reminding students to not only consider the value of a material and/or device for the wealthiest people in the G20 countries but also to consider the value in disadvantaged and/or more remote societies."

What follows are three examples of this type of research being carried out at MRI.

ESTHER OBONYO: LOW-CARBON, DURABLE BUILDING MATERIALS FOR LOW-INCOME AREAS

Esther Obonyo, associate professor of engineering design and architectural engineering with an affiliation with MRI, is a co-recipient of one of the Materials Matter at the Human Level seed grants, working on a project to develop bricks made via the cold sintering process. Cold sintering enables bricks to be made at much lower temperatures than traditional brick firing, enabling bricks to be made from materials that cannot withstand high temperatures and therefore, would not normally be available as a building material. This could include mining waste repurposed as a building material, or the use of local materials that might not otherwise be useful for making bricks.

This is an excellent example of Obonyo's research, which includes the development of low-carbon building materials that are both durable in extreme weather conditions and affordable for the local community.

"We are deploying these materials, both in the U.S. and also in East Africa," Obonyo, who was raised in Nairobi, Kenya, said. "A lot of what I do has focused on how to make these materials more durable in hot and humid environments, and also environments that are prone to flooding and other moisture related extreme weather events."

A hotter climate requires innovation in building materials for low-income housing, such as organic roofing materials that can passively cool a building's interior, and improved ventilation of building via better housing design.

Credit: U.S. Army photo by Lt. Col. David Konop, KITGUM, Uganda (CC by 2.0)

“We need materials that can help regulate the heat gain during summer days, and this is a global problem,” Obonyo said. “It does not matter whether you are in a Western country or in a developing country, extreme heat is a problem. Within the context of low-income communities, both here in the U.S. and in developing countries, they either cannot afford to lower the temperatures using mechanical devices or in many cases, they do not have access to those devices. So, these humanitarian materials can help regulate this temperature.”

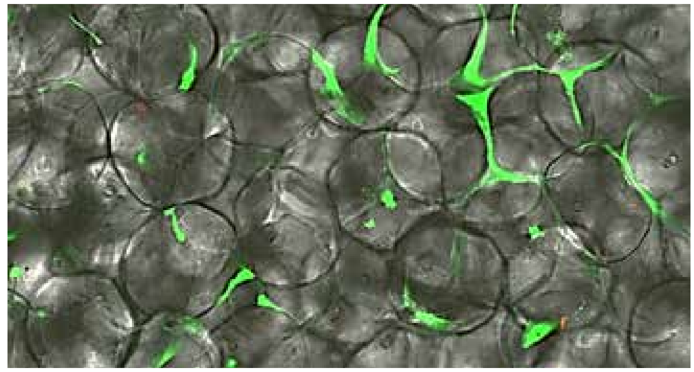
Such materials are lower cost to make, cheaper than materials that require welding. The price of welding as a percentage of total building envelope can range from 40% to 70%, contributing significantly to the price of housing. Obonyo and her lab are working on types of materials that do not require welding, such as bricks that can be made from local materials and studying the microstructure of these materials to create better and lower-cost bricks.

"We strongly believe that if we can significantly lower the price, through promoting the use of locally available resources, we can help bridge some of the gaps that exist with lack of access to adequate affordable housing,” Obonyo said.

Durability is also something to be considered, Obonyo said, because materials that are considered non-traditional may be viewed negatively by occupants who equate high quality with the use of concrete or steel. In addition, with increased extreme weather, the materials need to be resilient to hold up against hurricane winds and floods.

AMIR SHEIKHI: BETTER WOUND HEALING FOR EVERYONE

Amir Sheikhi, assistant professor of chemical engineering and biomedical engineering (by courtesy) with an affiliation in MRI, focuses his research on solving some of today’s challenges in biomedicine and the environment by designing novel soft material platforms. Sheikhi is also one of the recipients of the Materials Matter at the Human Level seed grants, to help develop a low-cost, ready-to-use biomaterial to help under-resourced populations have better results with wound healing.



Fluorescence microscopy image of cells adhering to the assembled GelMA microgels and spreading among them in 3D. Credit: Sheikhi Group/Penn State

"We will develop a wound-healing platform based on converting tissue-mimetic microengineered hydrogel particles, known as microgels, into powder,” Sheikhi said. “The powder will enable the on-demand, expertise-free use of healthcare biomaterials that can be applied to wounds at any time and by anyone in remote areas, which may enable the developing countries to access wound care solutions more readily and effectively.”

Sheikhi is working with researchers at the Penn State College of Medicine to translate this technology into wound care for areas that do not have decent access to healthcare infrastructures. The wound-healing platform would not require any preparation before use and can be applied to wounds right after the injury, reducing the healing time and increasing the healing quality.

Sheikhi said that the goal of this research is to help reduce the rate of hospitalization

“The 2019 cost of injury in the United States was $4.2 trillion, according to a report in the Center for Disease Control’s Morbidity and Mortality Weekly Report,” Sheikhi said. “The costs include spending on health care, lost work productivity, as well as estimates of cost for lost quality of life and lives lost. If successful, our technology may improve the quality of life of millions of people in the world and reduce the cost and complications associated with current wound care platforms.”

This work, Sheikhi said, is just one way he envisions materials researchers can view their research through a humanitarian

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lens. He notes that materials are inevitable parts of everyday life and play pivotal roles in numerous societal aspects.

“Looking into the future, materials researchers may focus on the true "impact" of their research on society,” Sheikhi said. “We can focus on understanding the properties of current materials and discover new materials to protect the natural resources and ecosystems and to provide sustainable sources of food, water, and energy."

KOFI ADU: X-RAYS YOU CAN DO ANYWHERE

One of the research focuses for Kofi Adu, professor of physics, Division of Math and Natural Sciences, Penn State Altoona with an affiliation with MRI, is carbon nanotubes. These single-wall nanotubes have diameters measured in nanometers, have exceptional electrical conductivity, tensile strength, and thermal conductivity. Some are metallic and others are semiconducting. They have applications ranging from electronics to optics and recently, have been explored as a new form of x-ray.

"I look at applications of some of the work that I do in terms of humanitarian application,” Adu said. “One of them is to develop a very compact, simple, easy to use x-ray that is portable, so that they can be used anywhere even where there is no electricity. The idea is to use carbon nanotubes, which are particularly good electron emitters. This could have a significant impact on healthcare in remote areas.

"In developing countries, a rural hospital might just be a few rooms, but this is something that could be designed where everything is in the box,” Adu said. "You could open it up, set it up, load whatever object you want to x-ray, and then do the x-ray. And then when you are done, just fold everything back up. This would have a great impact in rural areas where there are no electricity or a very limited amount of electricity.”

Another humanitarian materials research project Adu is involved in is using thermoelectric materials to both gather water in arid regions and to cool rooms in hot regions. Thermoelectric materials have an interesting property where when an electric current passes through the material, one side cools and the other side heats.

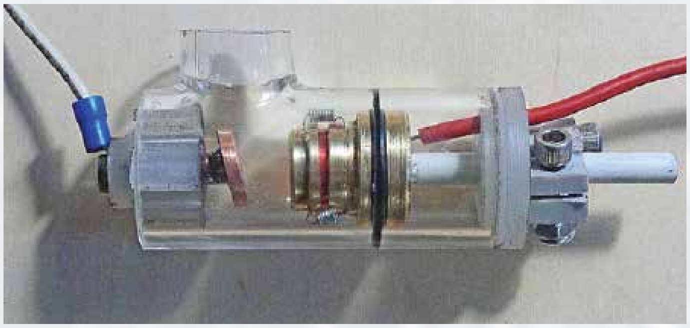
"You would be able to power this module with solar cells, and suck air through the cold end of the thermoelectric modules,” Adu said. “As you draw the air through the cold end, it condenses the moisture in the air into a tray that is drained out for use.”

An added benefit of this device would be to cool rooms with the air moved over the cold side of the modules.

“I'm originally from Ghana where it gets really hot,” Adu said. “It can also be hot at night inside the buildings even if the outside is cooler. This would have two major benefits if we are able to extract a lot of water from the environment while at the same time use the air from the device to cool the rooms.”

A model of this concept is currently being worked on by Adu’s lab.

“We designed a very compact version of it, but we couldn’t really work on this until now because of the pandemic, even though we had all the parts for it,” Adu said. “But now, I have students working on the project to create a module to see how well it will work.” ■



Prototype of CNT based X-ray tube.
Credit: Kofi Adu/Penn State

Increasing the impact of recycling through shared materials expertise

FOR MANY PEOPLE, recycling is just something you do as a good steward of the planet, taking the time to separate recyclables from the rest of your household garbage and then it is taken away on trash day, out of sight, out of mind.

Beyond protecting the environment, recycling also has deep, positive economic and employment impact for Pennsylvania. Credit: Adobe Stock

But what happens to these materials from the recycling bin to a product made from recyclables is a complex process, and one organization focused on getting the most out of secondary materials is the Pennsylvania Recycling Markets Center (RMC). Starting in 2020, the RMC began a partnership with Materials Research Institute (MRI) to work together to advance recyclable research via use of MRI's research resources and a series of research seed grants.

Founded by Penn State and as one of the University's affiliated corporations, the RMC is an independent 501(c)3 Non-Profit Pennsylvania Corporation housed at the Penn State Harrisburg with a mission of expanding and developing secure and robust markets for recovered secondary materials. Recycling is not just vital for protecting the environment, it also has a deep economic impact for Pennsylvania. As per the RMC, the act of recycling stimulates $50.9 billion in sales and supported more than 175,000 jobs in Pennsylvania.

"Since both RMC and MRI work with industry partners, we wanted to directly pair internal research capabilities directly with recycled materials industry outreach," according to Robert J. Bylone, Jr., President and CEO of the RMC.

Although the partnership is still relatively new, MRI and RMC are already working together on various projects. The Materials Research Institute serves as the link to materials research faculty and the RMC serves as the front-line connection to the recycling industry as well as manufacturers making recycled content products. MRI with RMC concurrence has funded five sustainable materials research projects in areas such as use of food scraps manufactured into degradable film plastics; recycled plastic used for the manufacture of graphite and graphitic compounds that are used in rechargeable lithium batteries; low-temperature sintering that allows the integration of unlike materials including waste materials; evaluation of recycled plastics in manufacture of durable goods; and evaluation of compounds in recycled plastics that could prevent chemical recycling of plastics.

The Recycling Markets Center is providing industry support; acquisition of experimental materials; curation and linkage to industry and material sortation experts; grant authorship support and review; provision of letters of support. Collaborative advertising is being developed such that "Design for Recycling" services can be leveraged as well.

For Bylone, these projects are just the beginning of a beneficial collaboration that will continue to pay dividends for the foreseeable future. ■

A hub with a lot of different spokes

MRI's centralized resources drives materials research, education across all of Penn State

Left. Chad Eichfeld, Nanofab director of operations Right. Joshua Stapleton, director of MRI's Materials Characterization Lab (MCL) Credit: Penn State MRI

DOING MATERIALS RESEARCH at the high level carried out by Penn State daily requires centralized facilities that serve all faculty, staff, and students across the entire University system from the Behrend Campus to the Brandywine Campus. Among the many benefits of this arrangement includes how such sharing of central facilities can lead to more contact and collaboration among researchers from different disciplines and units. Furthermore, the technical staff within these facilities provide invaluable expertise and support to the research community.

Which is one of the reasons why an interdisciplinary institute like the Materials Research Institute (MRI) is so important. The centralized facilities give researchers across all of Penn State access to facilities that they might not ordinarily have access to.

"It doesn't matter where you're coming from at Penn State to access these resources," said Joshua Stapleton, director of MRI's Materials Characterization Lab (MCL). "Which is something that I think the MCL takes pride in. We have a lot of good working relationships with the campuses, such as the Behrend College, the Dubois campus, the Altoona campus. It's in keeping with the exciting leadership and guidance of Penn State's Office of the Senior Vice President of Research, where they have created this commonwealth campus research program."

Stapleton is referring to the Commonwealth Campuses Research Collaboration Development Program (CCRCDP). The goal of this program is to support collaborative research projects between Penn State Commonwealth Campus faculty and the faculty and research staff at the shared core facilities at the College of Medicine and at University Park interdisciplinary institutes. There are seven of these institutes, of which MRI is one. Part of their work is to raise awareness of the availability of facilities like the one Stapleton operates.

"The CCRCDP program provides resources for commonwealth campus faculty to leverage university-wide research facilities like MCL" Stapleton said. "But the problem is a lot of Commonwealth faculty do not know about the resources. So how can they get access to it? And so that's kind of one of the drivers behind the program, to increase awareness like the MCL and put resources on the table for Commonwealth faculty."

As other stories in this edition of Focus on Materials have pointed out, characterization like what is done in the MCL is vital for materials research, and MCL's work shows up in these other stories. Along with supporting faculty research, the MCL also plays a key role in education at Penn State.

"MCL plays a key role in the applied characterization education of a very large number of students, and what I mean by applied is actually using tools to address problems," Stapleton said. "This includes how you prepare the samples, how you make the measurement, how you optimize the measurement, how you start to process the data, etc., which is different from just learning about the fundamentals via a textbook.

“Even though we are not currently running on any for-credit courses, MCL plays an important role in the hands-on education of students”

Another MRI facility playing a key role in cross-campus interdisciplinary research at Penn State is the Nanofabrication Lab (Nanofab), which has world-class capabilities in the areas of deposition, etch, lithography, material modification, and characterization. The number of materials the facility can process is impressive - more than sixty-five materials can be deposited and over seventy materials can be dry etched. It can handle both common materials and non-standard materials and is available to researchers in academia and in industry.

One commonwealth campus that Nanofab works with is Penn State Hershey. According to Chad Eichfeld, Nanofab director of operations, this has led them to work on some very interesting projects.

“Some of their faculty have developed some unique medical sensors and we have worked with them on their prototypes,” Eichfeld said. “The projects have lost a little steam during the pandemic given people down there are a little busy with other focuses right now, but I assume it is going to keep going since they are working both with us and other faculty on campus pulling those prototypes together.”

Along with the sensors, Eichfeld said they have offered support on some other cutting-edge medical research at Penn State Hershey.

"We've also done other things like over the years with Penn State Hershey, things like prototypes of artificial livers,” Eichfeld said. “The connection we have with Penn State Hershey has enabled us to work on some real outside-the-box kind of projects.”

Like MCL, Nanofab also helps with student research, helping the next generation of materials researchers gain the hands-on experience that enhances their education.

"While classes are great, as is learning from a book or from a paper, coming into a lab and actually ‘kicking the tires’ of how to actually do something is much different," Eichfeld said. “It's like someone working on their car. You can read a manual on how to change a head gasket, but when you get in there and do it, it's a much different job than what the book tells you. And it's the same for students here in Nanofab.”

Eichfeld said students from across the Penn State system encounter and learn to solve real problems in processing materials that they will encounter in doing research during their career. This is because often, they are doing work that has never been done before, so there is no manual to read.

"No matter what, you're going to encounter problems when you do something somebody has never done before,” Eichfeld said. “There's going to be problems and it's just about figuring out the source and making those connections on how you're going to solve that problem.”

“When a student starts, they come in green and they might not even know what a fab is, never set foot in one, but when they come out, they could probably be a tool owner in a fab,” Eichfeld added.

Whether it is a graduate student learning the ropes or a faculty researcher at another Penn State campus in need of state-of-the-art equipment for an experiment, Stapleton said that across MRI, the work they do is about being discipline agnostic. This means supporting research from different disciplines and helping Penn State faculty and students find the right tools to solve complex research problems.

"Academia can be great at creating silos, not interfacing with each other, and when that happens science loses out,” Stapleton said. “We don’t think like that, we think, okay, you got a microscale structure question. You got a nanoscale chemistry question. How can we help, how can we help you find an answer to your research questions?

“We run a research facility where it does not matter what discipline you are studying, if we have the right tools to address your question we are here to help” ■

Pushing biomedical materials research into the future

BIOMEDICAL-RELATED MATERIALS RESEARCH is a growing field that holds great promise. The impact that these new materials have already had on medicine and human health, such as tissue repair, prostheses, diagnostics, disease treatment, cancer research, and more, is significant.

Affiliated researchers in the Materials Research Institute are taking the science in exciting new directions in biomaterials and cancer research, working with the Penn State College of Medicine and Penn State Hershey.

Deborah Kelly, director of the Center for Structural Oncology, Huck Chair in Molecular Biophysics, and professor of biomedical engineering, often talks about how her work is figuring out how cancer “keeps outsmarting us.” Her focus on turning the tables and outsmarting cancer is built around structural oncology, which is better understanding cancer-causing processes through the study of the atomic scale of the proteins in cancerous cells.

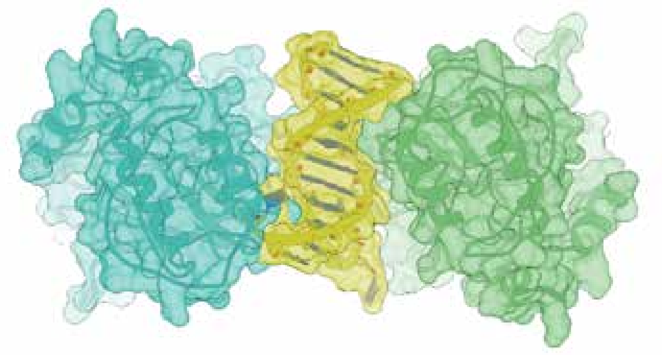
“My research involves a couple of different areas, one of which is cancer research and looking at different ways in which genetics affects the development of cancer, particularly breast cancer, as well as brain tumors and pancreatic cancer,” Kelly said. “This includes the molecules involved that enable either at the initiation of the disease or the progression of the disease, and we use high-resolution imaging technology to actually look at the molecules involved. We acquire the molecules from cancer cells, and we look at the healthy ones versus the unhealthy ones and then we try to infer what the differences are using atomic-scale modeling.”

Kelly’s research has led her to a new collaboration with George-Lucian Moldovan, associate professor of biochemistry and molecular biology at Penn State Hershey’s Penn State Cancer Institute.

“He and I are starting to work on projects in which we want to investigate these breast cancer susceptibility genes at a higher level,” Kelly said.

The goal is to recapitulate disease-related mutations in the gene and understand the outcomes. Moldovan's lab can do modifications to the gene sequences using gene editing technology in cells in the lab. With these gene editing technologies that recapitulate the mutations seen in disease, they can start to understand on a deeper level how these all these disease-related mutations can affect the normal function of proteins, and also who they can be corrected in the cells in which they are being produced.

"We want to apply CRISPR gene editing tools to mimic how these cancer cells form in culture dishes, then study how these effects are related to patients’ cells,” Kelly said. “By using modern editing technology we hope to understand the underlying disease processes.”



Structural model of the p53 tumor suppressor protein engaging DNA. Credit: Kelly Lab

They will also work on the protein p53, which is a tumor suppressor.

"P53's normal job is to prevent tumors from happening and when it's mutated and becomes dysfunctional, then cancer can be propagated or progressed and some cancers thrive on the fact that it doesn't have something sort of regulating its DNA the way it should be normally," Kelly said. "And so we're doing structure-related 3D modeling on what these proteins look like as well."

Deb Kelly professor of biomedical engineering and director, Center for Structural Oncology, focuses on figuring out how cancer "keeps outsmarting us." Credit: Kelly Lab

While this is still in the planning stages, Kelly is already excited about the potential. She also sees it as the type of collaboration that is necessary for moving cancer research in new directions.

"I think using these editing technologies to recapitulate disease at a deeper atomic level really represents the benefits of the idea of convergence between life sciences and materials research, using the high-resolution imaging as well as some of the biology tools that's in the works," Kelly said. "We've already got the tools and the imaging technology in place. We're hoping to launch this new initiative with the Moldovan lab very soon and we want to eventually roll this out into the Penn State community as a CRISPR Cancer Consortium through the Next-Generations Research Program at the PSCI."

With biomaterials, an example of the work MRI is doing with Penn State Hershey involves research by Dino Ravnic, staff physician at Penn State Hershey, and MRI-affiliated faculty. One is a new type of bioadhesive glue that will facilitate tissue reintegration by preventing seroma formation. Seromas are a collection of fluid that builds up under the surface of the skin.

"Seromas after any kind of surgery are commonplace and an issue," Ravnic said. "We've developed an abdominoplasty model in a pig and are testing the bioadhesive glue to see if seroma accumulation can be mitigated and if tissue integration can be improved."

A method that drastically reduces the number of seromas in surgical patients would be a significant benefit for patients, as current methods for dealing with seromas could use improvement, Ravnic said.

"What we do now to remove unwanted fluid after surgery is to put drains in place," Ravnic said. "The drains are cumbersome for patients, and they don't work all the time. There have been a variety of different kinds of materials developed that try to reattach the disrupted tissue planes following surgery, but none have truly been successful. So there exists a great void in this space."

The bioadhesive glue has an advantage in that a simplified version of it is already FDA (Food and Drug Administration) approved for other uses.

"Because of this, I think this bioadhesive glue can be clinically translatable pretty quickly," Ravnic said.

Ravnic added that research such as his and Kelly's benefit from the diversity of perspectives that university-wide collaborations enable.

"The University functions better when there are collaborative approaches across campuses, and that's the take-home message," Ravnic said. "The things that are being done in material research are vital to advancing clinical medicine. Therefore, I think it's really instrumental that these partnerships exist, and it's great that we're able to carry out this research underneath the Penn State umbrella." ■

Better plastics and sustainable supply chains drive Behrend materials research

PLASTICS, SUPPLY CHAIN, and sustainability may seem like an odd combination, but they all play a role in making Penn State Behrend a unique resource for materials research at Penn State.

Penn State Behrend is home to the Plastics Engineering Technology program and the Plastics Engineering Laboratory. Now in existence for more than 30 years, the bachelor's degree program is highly regarded, with more than 1,200 graduates, and is one of the few accredited programs of its type in the country.

Research areas for Behrend faculty and students include plastic part design for disassembly, additive manufacturing, and plastics property optimization. Behrend's research in plastics processing uses some of the best processing equipment in the world such as MuCell microcellular foaming, compounding, extrusion, film processing, injection molding, and formulation lines. In addition, extensive research is performed in plastics recycling, melt rheology, polymer crystallization, and composite formulation for high-performance applications.

In essence, Behrend researchers are revisiting and revitalizing old fields of study and putting a new spin on them.

"It's like that old song, everything old is new again," said Alicyn Rhoades, interim associate dean for research and graduate studies at Behrend and associate professor of engineering, plastics engineering technology, and polymer engineering and science programs. "The polymers that comprise commodity plastics are not known as sexy and beautiful. In the 1980s, the materials science community basically decided that they were done researching those materials, moving on to more exotic and exciting polymer systems.

"But with recent advances in characterization instrumentation, including the tools we have developed at Penn State, you can turn around and do a lot of good with polymers that are, broadly speaking, important to society," Rhoades said. "We have revisited the physics of these basic materials and have been able to move the needle on interesting research that changes the way plastics are engineered."

Along with being a hub for plastics research, Behrend is also the U.S. home of the Advanced Resource Efficiency Center (AREC USA), an organization that promotes collaboration between industry and universities to meet sustainability challenges across supply chains. AREC was founded by the University of Sheffield in Great Britain, and from this central location, has "spokes" in the form of AREC Europe, AREC China, AREC USA at Penn State Behrend, and a new AREC spoke that will be announced soon. AREC USA is directed by Rhoades.

"AREC is designed to help us look at new technologies and science and be able to ascertain whether it has long-term potential, whether it has long term sustainability impacts, whether it's a positive thing for the planet, and what new regulations may come down the pike that would affect it," Rhoades said, "and also, whether it will ultimately fail because it's bad for the planet. We look at environmental factors, we look at cost, and we look at the big-picture reality of taking new technology to market and how it might affect existing industry."

AREC USA incorporates two institutes based at Penn State University Park, the Materials Research Institute (MRI) and the Institute of Energy and the Environment (IEE), and the Plastics Engineering Laboratory at Behrend, forming a

Credit: Matthew Warner, Class of 2007

unique cross-campus collaboration within the larger partnership with the University of Sheffield. This partnership enables a more complete characterization of a material, according to Gamini Mendis, assistant professor of engineering, plastics engineering technology, and polymer engineering and science programs at Behrend.

"I use MRI's characterization facilities for a lot of hands-on plastic projects to understand the structure-properties relationships of those materials," Mendis said. "The AREC center is really useful because, when you are going to MRI for characterization, you are looking at material properties that let you know whether something will be good as a product, but there is really no way to quantify sustainability in a lab. You cannot look at embodied CO_2 emissions by throwing a material into an x-ray diffractometer or in an SEM (scanning electron microscope)."

The AREC center, Mendis said, enhances the ability to characterize materials by looking at the sustainability footprint using a technique called life cycle analysis (LCA), which breaks down the production of something into useful unit processes. Doing this enables researchers to look at the materials that go into each of those unit processes and the associated carbon emissions, energy emissions, or energy consumption from each of those inputs. This quantifies the CO_2 footprint of a product or a process.

"This is really useful for decision making," Mendis said. "If you are trying to commercialize new products, and you really want to be marketed as green, you need some numbers to back that up. And maybe in developing this product, you have incorporated accidentally a couple of processes that have a high CO_2 footprint. By doing this quantification, we can target the parts of your process that you might want to change or research new solutions to lower the overall impact of the product or process that you are developing. It is really a tool to better understand the sustainability of your material."

AREC USA's first big project was with the Advanced Research Projects Agency - Energy (ARPA-E), developing a tool related to the transport of municipal solid waste and recycled recycling materials. Behrend researchers in AREC USA used publicly available data from two different municipal waste sites, one in West Palm Beach, Florida, and one in York, Pennsylvania.

"All of their waste handling data is publicly available, and they have waste-to-energy at both places," Rhoades said. "Based on the economics and the logistics data, we were able to make baselines using real data in two very different parts of the country. And then ARPA-E can use that tool to assess the practicality of some of these technologies that might come to influence the end-of-life cycle of materials."

For example, the tool can be used to determine whether a new recycling technology is reasonable from an energy point of view, or whether the logistics of moving plastic waste make sense.

"The model in this tool accounted for how far the trucks had to go, the tipping fees, and all the things that have to do with waste processes that are just not things that scientists usually think about," Rhoades said. "They do not think about, you know, the 40 cents we might save on this or how much CO_2 we might save via using this process—just looking at the energy balance of the big situation. We did that for ARPA-E and that was pretty successful."

The societal impact of these activities is what drives AREC USA's goals as an organization, according to Mendis.

"We're trying to create a real circular economy here, trying to close materials loops and get materials that would end up in the landfill into new homes and applications," Mendis said, "so that way you do not create all that waste. There are a lot of studies asserting that any time we throw something in a landfill, it disproportionately affects marginalized communities. By preventing materials from ending up in the wrong place, we're minimizing those effects." ■

Penn State DuBois partners with MRI to become powder metal/additive manufacturing hub

IN PARTNERSHIP WITH the Materials Research Institute (MRI), Penn State's DuBois campus has become a center for the growing field of additive manufacturing and powder metals, charting out a new course for impactful metals research.

DuBois is located in northcentral Pennsylvania, which during this century has become a hub for the powder metallurgy industry. As per the St. Mary's, Pennsylvania Chamber of Commerce, roughly 40% of the world's powder metal parts are produced in Northcentral Pennsylvania, employing over 10,000 people at more than 50 firms.

The region's leadership in this field makes MRI and Penn State Dubois joint research efforts a logical partnership. This includes working with Penn State DuBois faculty members, such as Ram Rajagopalan, associate professor of engineering and affiliated member of MRI, who in turn partners with MRI-affiliated faculty at the University Park campus, such as Amrita Basak, assistant professor of mechanical engineering.

Rajagopalan's research focuses on surface metal modification of powder metals, including a process known as cold sintering developed by Clive Randall, director of MRI and distinguished professor of materials science and engineering. Cold sintering is an innovative ultralow temperature sintering process that is used in ceramic production. In collaboration with Randall, Rajagopalan has researched how this process may be extended to powder metals.

This process would potentially improve the green strength, or handling strength, of steel, an important property in powder metal manufacturing that determines the productivity rate and yield of the powder metal components. High green strength also enables green machining, which is machining to shape the metal or ceramic bodies prior to the sintering process.

"The green strength is enhanced to such an extent that you could actually do green machining now, and green machining is a very interesting concept," Rajagopalan said. "First of all, you could use green machining to develop or fabricate complex shapes using powder metal. And secondly, you could significantly reduce the tool wear because without green machining, after you sinter the powder metal parts, you will have to do some kind of secondary machining."

Along with the sintering of powder metals, Rajagopalan partners with MRI for research on the development of carbon materials for energy storage applications. Potentially impactful applications of this research include wearable, self-powering health monitors. "My main focus has been on developing low self-discharge electrochemical capacitors," Rajagopalan said. "Electrochemical capacitors are energy storage devices, just like batteries, but they are traditionally viewed as high-power devices and one of their weaknesses is energy density."

Through this project, Rajagopalan and his lab have increased the energy density of the electrical super capacitors by almost three to four times. "When you push the energy density up and combine with the high cycle life capability and high-power performance of these capacitors, you can think of using these devices either as a standalone energy storage device or in conjunction with batteries for many applications," Rajagopalan said. "One such application was the wearable health monitoring device where we demonstrated that you could actually make a self-powered system for continuous monitoring."

Basak works with additive manufacturing, which is industrial-level 3D printing, perfecting the process to create materials that are free of defects such as cracks.

"I say it's like cooking as that is the best example since everybody knows cooking," Basak said. "You must figure out what would be the best recipe so that the final dish is up to your satisfaction. So, my research is mostly related to that; I try to find the best recipes to process high-strength materials so we can make good parts. We use advanced modeling, machine learning, and characterization tools to accelerate the process of developing these recipes."

This type of "cooking" to get the right "recipe" could mean avoiding defects at the micron scale, something that requires sophisticated characterization techniques and equipment, such as scanning electron microscopes, EDS x-ray spectroscopy, and microhardness measurements. This is where MRI's Materials Characterization Lab (MCL) facilities at the Millennium Science Complex on Penn State's University Park campus play a significant role.

Basak gave two examples of projects she is working on; one is with NASA and the other is with the U.S. Army. With the NASA project, she is working to optimize designs for cooling holes to improve the overall efficiency of the engines.

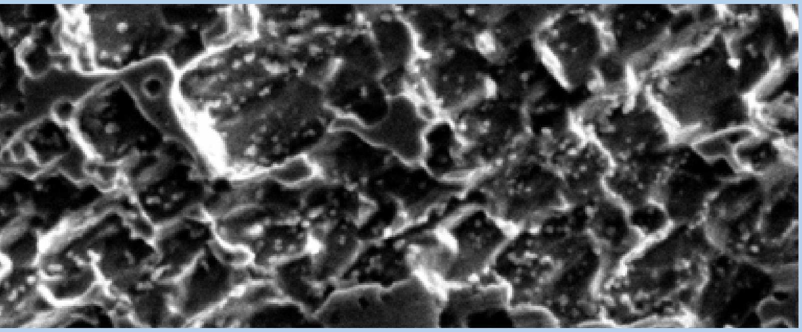
"The NASA project researches how you can make really efficient cooling holes with additive manufacturing," Basak said. "MRI's characterization facilities are particularly important here because we have to make the parts and then cross-section them to see whether we are able to print what we actually intended."

With the U.S. Army, Basak and her lab are working on high-strength steels that are of interest to the Army.

"The steels used in various army-relevant applications possess very high strength, and we are looking at how to make them with additive manufacturing," Basak said. "So again, we are trying to cook the recipes, so that the part we are making has these high strength properties. And like in the NASA project, characterization like what MRI offers is vital for qualification."

Testing and characterization at such a high level is something that Basak said would not be possible unless there was a central facility like MRI's.

"The MRI facilities are essential for metal research," Basak said. "Imagine the scale of that equipment and the amount of maintenance they require. Without a centralized facility, it would be very hard for an individual investigator to have those facilities in his or her lab right, almost impossible. MRI is so important because materials characterization is the heart of metal research." ■



Microstructure of an additively manufactured nickel-base superalloy specimen observed with a scanning electron microscope. Credit: Amrita Basak

Adding collaboration to additive manufacturing research at Penn State

ESTABLISHED IN 1945 at the request of the U.S. Navy, the Applied Research Laboratory (ARL) was originally focused on developing technology related to undersea systems. Today, ARL has a broad research portfolio that includes materials and manufacturing research, and partners with Materials Research Institute (MRI) on a variety of projects.

The partnership with MRI came naturally, according to ARL's Edward "Ted" Reutzel, given how many of these projects are materials related. One example is a strategic effort that focuses on additive manufacturing—essentially 3D printing at an industrial scale—to enable the efficient fabrication of parts that can offer any of a range of benefits, such as enabling optimized designs that are lighter than designs constrained by traditional manufacturing processes..

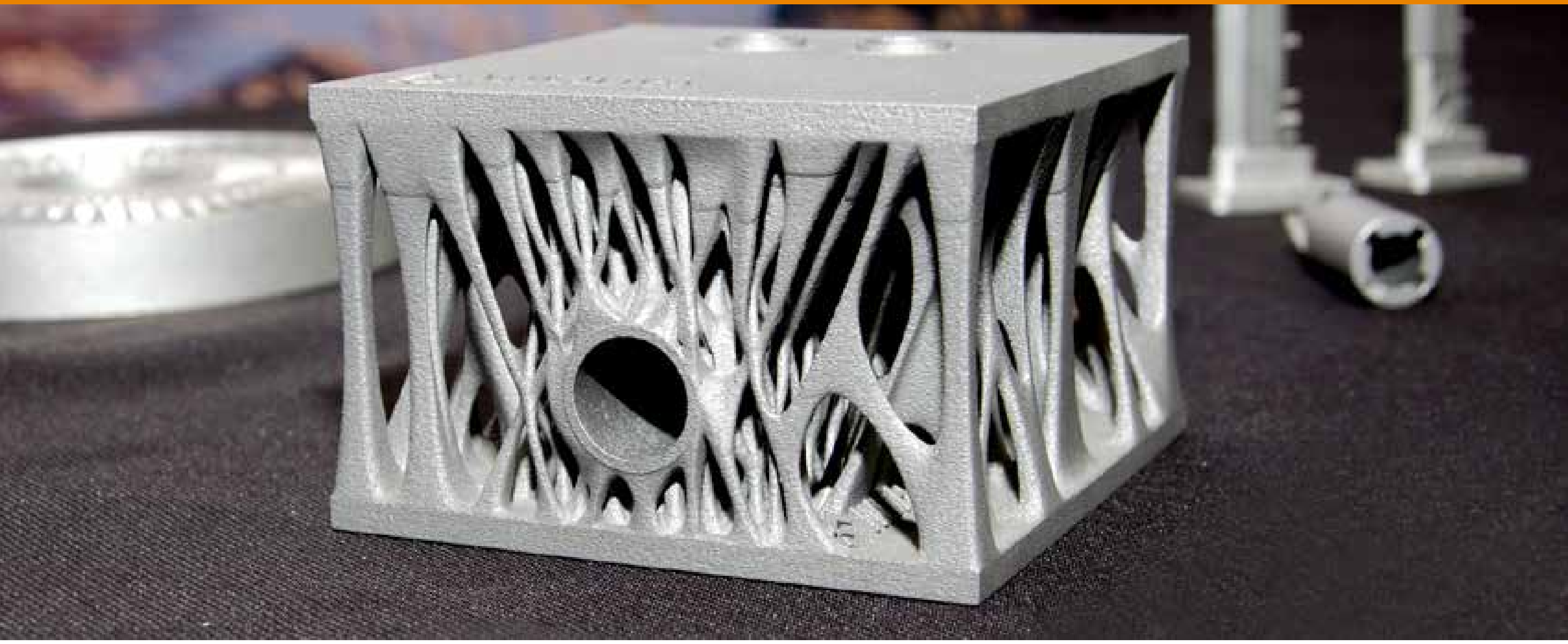
Reutzel is one of three co-directors of the Center for Innovative Materials Processing through Direct Digital Deposition (CIMP-3D) and associate research professor with ARL. CIMP-3D's mission is to enable interdisciplinary research that discovers, develops, and deploys metal-based additive manufacturing technology for critical applications.

"CIMP-3D is a University-wide activity that's largely operated by ARL," Reutzel said. "The way it was developed, there are actually three directors, the primary director responsible for operations from ARL, and then there is a co-director, Professor Tim Simpson, who represents the College of Engineering, and who was the first Director for Penn States Additive Manufacturing and Design Graduate Programs, and a co-director representing the Department of Materials Science and Engineering, Professor Mike Hickner, who also serves as an associate director at MRI. It's extremely helpful to have such broad representation because additive manufacturing is such a highly multidisciplinary activity. CIMP-3D is designed from the ground up to foster that kind of multidisciplinary teaming, and that naturally leads to a lot of interaction with institutes at Penn State like MRI."

Along with regular meetings to plan collaborative projects among the three directors, CIMP-3D has assembled a group of more than 50 faculty associates who do additive manufacturing research across the Penn State system. The Center is a shared facility, where ARL operates the metal additive manufacturing machines and Hickner oversees polymer systems. A key role for MRI in this work is to support advanced characterization of the additively manufacturing materials, and MRI's facilities in the Materials Characterization Lab are vital to the process.

Among additive manufacturing's critical applications include building components such as hydro generators and flight-critical components for aircraft. Often, conventional manufacturing technologies produce a lot of waste, and Reutzel gave the example of "buy-to-fly ratio," which is a term referring to how much material you need to buy and machine away to have a component that flies.

"In some cases, for more advanced aircraft, to create a component within the airframe, they have to start by buying a huge block of material," Reutzel said. "They end up machining away 90% of that material. That's a lot of wasted material



Complex metal parts made by additive manufacturing in the CIMP-3D. Credit: Penn State

and there are environmental impacts associated with it. With additive manufacturing, you can build something that's near net shape, so there can be significantly less wasted material."

Reutzel gave another example of how additive manufacturing can have positive societal impacts: The ability to repair components that before could not be repaired and therefore had to be replaced, such as a titanium drive shaft that corrodes and wears on the bearing surfaces. Such a component has high value not just because of the expensive material, but due to the amount of work that goes into manufacturing, so being able to repair it is important. However, it cannot be repaired with typical arc welding techniques because the heat distorts it and makes it unusable.

"With additive manufacturing, you can make repairs with much less heat input and less distortion, and therefore, you open up a whole new realm of possibility for repair," Reutzel said. "So rather than throw that part out and build a new one, you can conceivably repair it, inspect it, and put it back in use for much less money, with much less time delay, while using fewer resources."

ARL partners with MRI to help advance a wide array of related technologies, such as a mobile robot repair system for industrial use that can perform arc weld, cold spray, or laser-based repairs and even do inspection and final machining, all in one system.

"It's worth noting that for research involving material science and manufacturing technology, having ARL as an integral part of Penn State can be a big benefit," Reutzel said. "ARL helps make Penn State unique in our ability to both perform the fundamental research, and then bridge the technology 'valley of death' to help make new science and technology an industrial reality. MRI is a critical part of that because the materials characterization capabilities and expertise the Institute offers are second-to-none, and really highlight the benefits of working with Penn State." ■

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