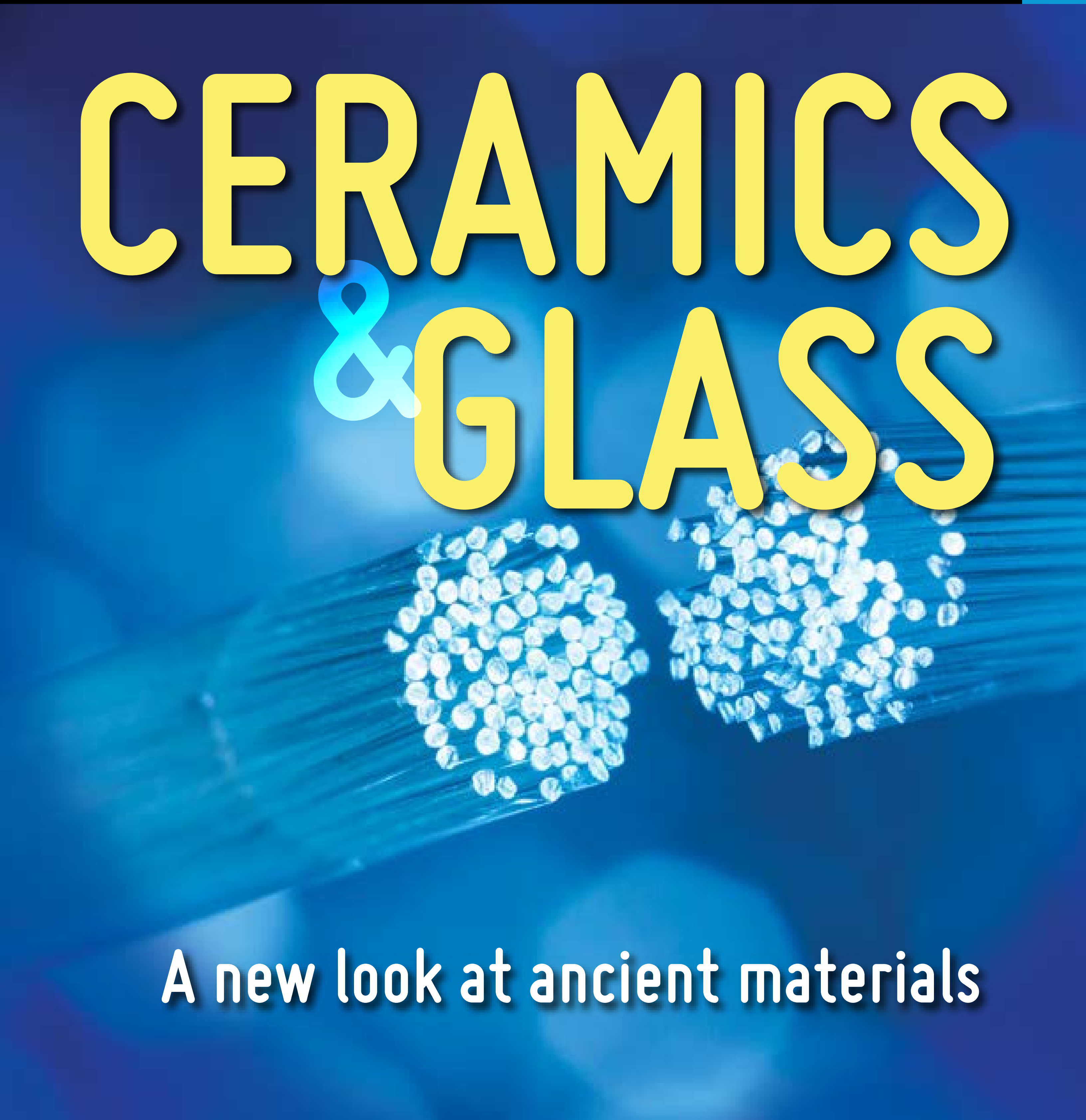
Penn State Materials Research Institute

FOCUS on MATERIALS

MATERIALS RESEARCH INSTITUTE MAGAZINE

SPRING 2023



CERAMICS & GLASS

A new look at ancient materials

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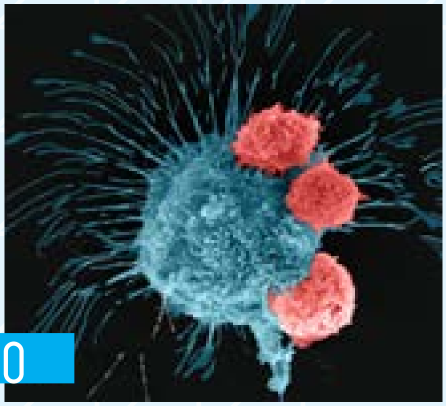

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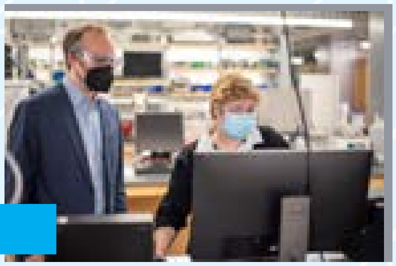

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FOCUS on MATERIALS

MATERIALS RESEARCH INSTITUTE BULLETIN

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

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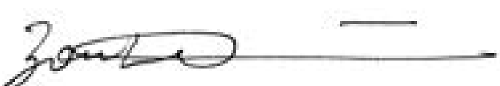
From the Acting Director

I am Zoubeida Ounaies, acting director of the Materials Research Institute (MRI), professor of mechanical engineering, and director of the Convergence Center for Living Multifunctional Materials Systems. I am thrilled to contribute this Director's Message while Clive Randall is away on sabbatical.

In this issue, we highlight Penn State's research in ceramics and glass, two materials that are both incredibly old and yet replete with new possibilities ripe for exploration. Humans have made ceramics for at least 25,000 years, and glassmaking dates back at least 6,000 years. We, in the Materials Research Institute (MRI) and at Penn State, have long been at the forefront of innovation in glass and ceramics. While conventional uses of glass for windows and ceramics for pottery are well-known, glass and ceramics have so much more to offer than those "traditional" applications.



Zoubeida Ounaies
Acting Director
Materials Research Institute

In 1923, Penn State established the Ceramic Science program, one of the first such programs in the nation. In our Pioneers of Materials Historical Poster Project that adorns the walls of the second floor of the Millennium Science Complex, ceramic research trailblazers such as L. Eric Cross, Della Roy, Rustum Roy, and Robert Newnham are prominent. On the glass side, past leaders in research including Carlo Pantano (former director of MRI) and Wondemar Weyl are also represented and celebrated.

These amazing people rethought the potential of glass and ceramics, branching out into developing new applications for these materials that many people might find surprising, such as glass for safe long-term immobilization of nuclear waste and ceramics for energy storage. These fields of research helped MRI progress from its roots as the Materials Research Laboratory founded in 1962, into MRI's founding in 1992. Today, MRI is an interdisciplinary materials research powerhouse, with more than 320 faculty members and 150 researchers from 15 departments and five colleges across Penn State.

The word interdisciplinary is key to our success. We do not do silos in MRI. We facilitate and promote diversity of thought and fields, bringing people together to advance amazing research. I am passionate about this research, and I strive to advance diversity, not just in fields of study but also in recognizing the richness of contributions of researchers from traditionally underrepresented groups. On March 31, 2023, MRI, along with Penn State's Department of Materials Science and Engineering, held a Women in Science Luncheon as part of Women's History Month, to honor the contributions of giants in science at Penn State such as Dorothy Quiggle, Della Roy, Pauline Mack, and more.

These women inspire me. They are legends of the past whose legacy we strive to uphold. They are inspiring a new generation of researchers who are exploring glass, ceramics, and other materials to tackle societal grand challenges such as the urgency of climate change and the search for silicon's replacement for future semiconductors. Some of these great Penn State women researchers are featured in this very issue, such as Susan Trolier-McKinstry, Aida Ebrahimi, Amrita Basak, Shadi Nazarian, and Jun Zhu, just to randomly choose a few.

The widely accepted traditional view of what a scientist looks like continues to fade as a new generation of researchers expands the boundaries of research at MRI. Like glass and ceramics, they defy outdated expectations as they author the next chapters of materials research at Penn State.

Amrita Basak, assistant professor of mechanical engineering at Penn State, will use her Defense Advanced Research Projects Agency Young Faculty Award to create computational models to predict ways in which parts created with a nickel-based material known as Inconel Alloy 625 may become warped during the additive manufacturing process. Credit: Kelby Hochreither/Penn State

ENGINEER EARNS DARPA YOUNG FACULTY AWARD FOR MULTI-LASER ADDITIVE MANUFACTURING

By Sarah Small

AMRITA BASAK, ASSISTANT professor of mechanical engineering at Penn State, has received a two-year, $498,235 Defense Advanced Research Projects Agency (DARPA) Young Faculty Award for her work predicting and preventing thermal deformation in multi-laser additive manufacturing (AM).

The DARPA Young Faculty Award, according to the program's website, identifies "rising stars in junior research positions … [to] develop the next generation of academic scientists, engineers, and mathematicians who will focus a significant portion of their career on [Department of Defense] and national security issues."

Basak will use the award to create computational models to predict ways in which parts created with a nickel-based material known as Inconel Alloy 625 may become warped during the AM process. These predictions would allow researchers to calibrate the AM equipment accordingly to prevent these flaws. She focuses on an AM method called laser powder bed fusion and, specifically, how to use multiple lasers at once to build parts in layers, taking far less time than single-laser AM.

To make accurate predictions about potential deformation, Basak said the project requires input from researchers from multiple fields, including manufacturing, computational modeling, and artificial intelligence.

Based on the specifications of the laser powder bed fusion technique and the desired material, Basak will first develop numerical models to predict potential deformation. Next, she will work to improve the process with scan optimization. This type of computational work helps identify the optimal parameters in a given simulation, such as the best pathways for multiple lasers moving simultaneously.

A person could consider their various options to decide to fly, and a search engine could produce possible flights based on specific dates and locations. But there are still so many potential

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choices that could result in an optimal or less-than-ideal journey. Scan path optimization for additive manufacturing helps set the best path and produce the best outcome — in this case, minimum deformation.

"This is an example of high risk, high reward research," Basak said. "The field of predictive computational modeling for scan path optimization is still nascent for powder bed fusion AM with one laser, let alone multiple lasers. This work is so new that there are ample opportunities to fail, but also, if it works, we will be able to contribute something entirely new to the literature."

Basak said that the mentorship she has received at Penn State was what ultimately encouraged her to pursue such a challenging project. She specifically credited former DARPA awardee Tak-Sing Wong, professor of mechanical engineering and of biomedical engineering and is affiliated with the Materials Research Institute, as well as Tim Simpson, Paul Morrow Professor in Engineering Design and Manufacturing, and Ted Reutzel, director of the Center for Innovative Materials Processing Through Direct Digital Deposition, who offered advice throughout the application process. She also recognized the guidance of her department mentor, Zoubeida Ounaies, professor of mechanical engineering, acting director of MRI, and director of the Convergence Center for Living Multifunctional Material Systems. ■

EVENT LIFTS CURTAIN ON A BRIGHT FUTURE FOR MATERIALS RESEARCH

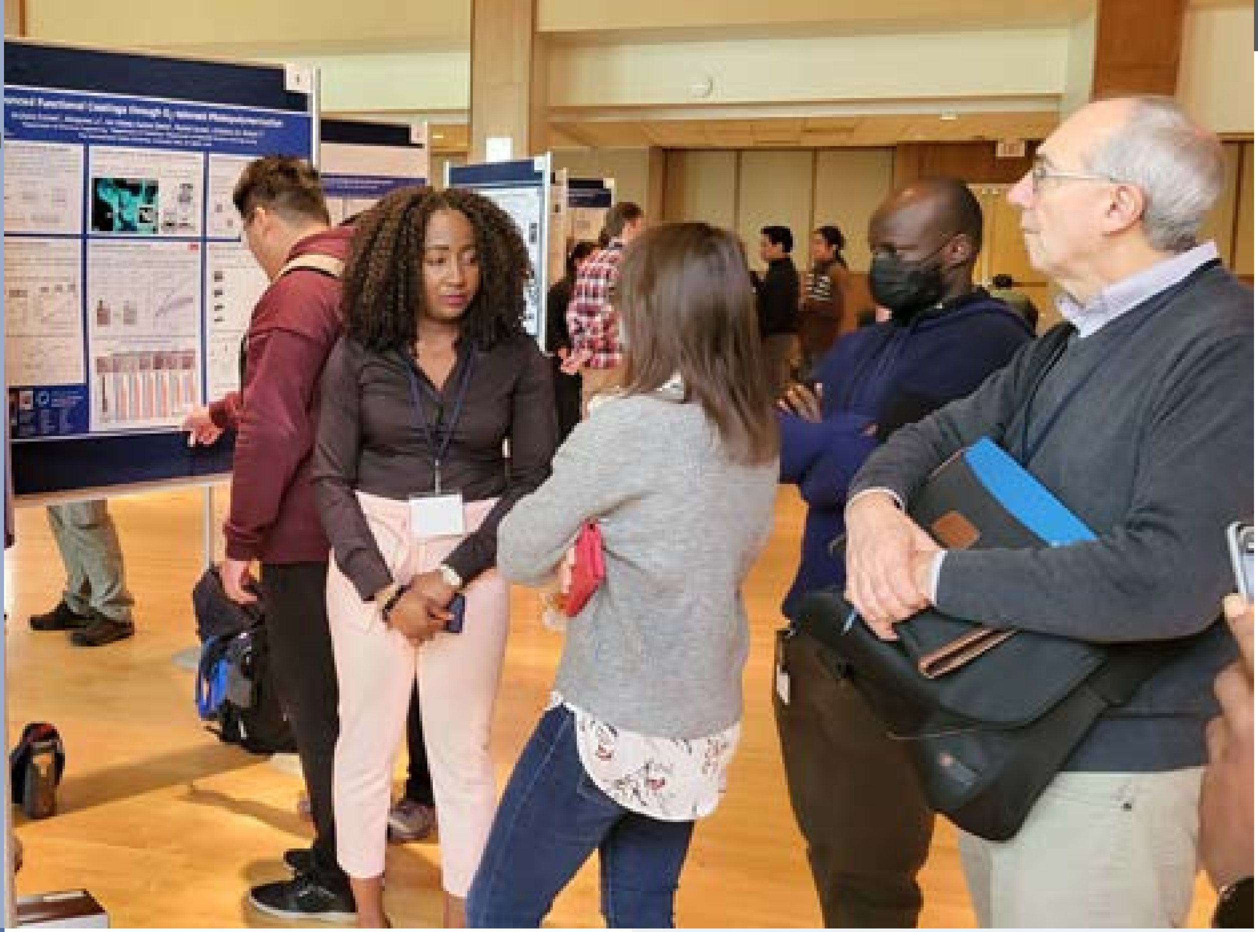
By Jamie Oberdick

YOU ARE READING this because of materials.

Whether you are perusing this article on an electronic device driven by a semiconductor chip or via a paper printout, the ability to read these words is in a large part due to innovative materials research that led to a product in use in society. And the future holds more innovation in materials research, including at Penn State. The 2022 Materials Day event, presented by the Materials Research Institute with the theme "Materials Impacting Society," featured a look at what might be on the horizon as far as materials research with positive societal impact.

The event was held in October 2022 on the Penn State University Park campus and was attended by more than 300 materials researchers from Penn State, industry, and government. The event featured keynote speakers, breakout sessions, the presentation of the 2022 Rustum and Della Roy Innovation in Materials Research Awards, and networking events. All of these had one thing in common: Discussion of what continues to be a very bright future for materials research at Penn State and beyond.

"Every aspect of modern civilization has relied upon having the appropriate materials available to enable those advances," said John Mauro, Dorothy Pate Enright Professor and associate head for graduate education in the Department of Materials Science and Engineering, who gave one of the

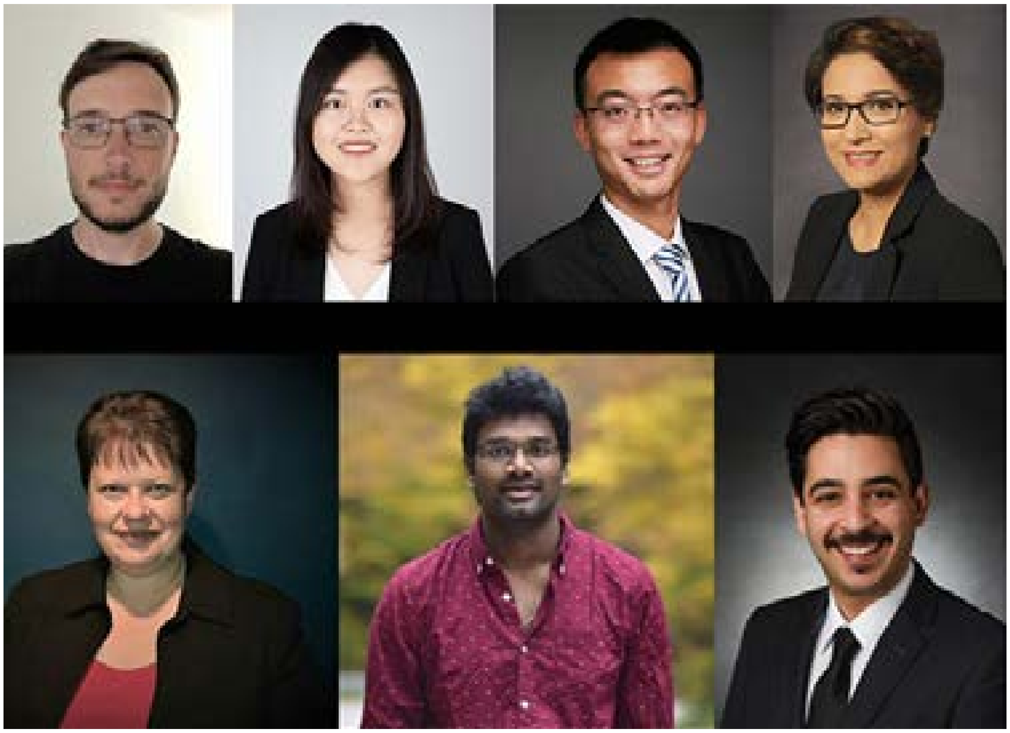


Materials Day attendees gather for one of two poster sessions at Alumni Hall in the HUB-Robeson Center on the University Park Campus on Oct. 20. Credit: Jamie Oberdick/Penn State

keynote addresses that focused on the United Nation's International Year of Glass and trends in glass research. "Materials science and technology are key in addressing global challenges in energy, the environment, information technology, healthcare, transportation, sustainability, and more."

Another point of discussion for Materials Day was the CHIPS and Science Act, which was signed into law by President Joe Biden in early August 2022. The law is designed to jumpstart America's semiconductor industry so that it regains its share of the global market, including the development of regional hubs via partnerships with industry, government, and other universities. This is also poised to inject millions of training and research dollars into growing the semiconductor workforce and supply chain, which is good news for Penn State given how well the University is positioned in materials research and workforce development.

"Materials Day is a unique opportunity to meet other materials researchers at Penn State, to network and have students learn about emerging research that they might not otherwise know about," Zoubeida Ounaies, MRI acting director, professor of mechanical engineering, and director of the Convergence Center for Living Multifunctional Material Systems. said. "In fact, graduate students in my research group ended up reaching out to colleagues they met at Materials Day to explore possible collaborations and to learn about their approaches." ■



Clockwise from top left, Fabien Grisé, Kunyan Zhang, Lin Wang, Aida Ebrahimi, Amir Sheikhi, Akhil Dodda, and Nichole Wonderling

MATERIALS RESEARCH INSTITUTE NAMES 2022 ROY AWARD WINNERS

By Jamie Oberdick

SEVEN PENN STATE materials researchers have received the 2022 Rustum and Della Roy Innovation in Materials Research Award.

The award is presented by the Materials Research Institute and recognizes interdisciplinary materials research at Penn State that yields innovative and unexpected results. The award has expanded this year to include four categories: Junior Faculty, Non-Tenure Faculty and Research Staff, Post-Doctoral, and Graduate Student. The award exists thanks to a gift from Della and Rustum Roy, who are both late alumni of Penn State's College of Earth and Mineral Sciences and long-serving faculty in the college.

This year's winners were announced at the 2022 Materials Day event in October. They include in the Junior Faculty category, Aida Ebrahimi, Thomas and Sheila Roell Early Career Assistant Professor of Electrical Engineering and Biomedical Engineering, and Amir Sheikhi, assistant professor of chemical engineering and biomedical engineering (courtesy). In the Non-Tenure Faculty and Research Staff category, the winners include Nichole Wonderling, X-ray scattering manager, Materials Research Institute (MRI), and Fabien Grisé, associate research professor of astronomy and astrophysics. In the Post-Doctoral category, the winner is Lin Wang, postdoctoral scholar in mechanical engineering, and in the Graduate Student category, the winners include Akhil Dodda, engineering science and mechanics doctoral student, and Kunyan Zhang, doctoral candidate in electrical engineering. ■

Amir Sheikhi and Aida Ebrahimi

Amir Sheikhi

Sheikhi's multifaceted research via his Bio-Soft Materials Laboratory (B-SMaL) focuses primarily on micro- and nano-engineering of natural or semi-natural materials to develop functional soft matter/biomaterials with tailored structure-property relationships for health care and environmental applications.

Kunyan Zhang

Zhang's research focuses on improving the sensitivity of biological sensors using nanomaterials for early detection of life-threatening medical conditions that enables best-case treatment options and increasing survival rates.

Kunyan Zhang and Clive Randall

Awards presented by Dave Fecko, Director of Industry Collaborations and Clive Randall, Director of MRI Credit: Seana Wood/Penn State

Aida Ebrahimi

Ebrahimi's research revolves around advancing biosensors and bioanalytical platforms for health monitoring through a multidisciplinary approach which involves materials and device engineering, devising novel sensing modalities, and convergence with advanced data analytics.

Dave Fecko and Fabien Grisé

Akhil Dodda

Dodda's doctoral research focused on implementing energy-efficient optoelectronic systems for sensing, storage, computing, and developing novel security primitives using two-dimensional materials. This research would help to meet security/privacy needs in the rapidly evolving digital era, such as a smart and secure Internet of Things.

Nichole Wonderling

In Wonderling's current role as manager of the X-ray Scattering facility in MRI's Materials Characterization Laboratory, she manages the operations of the lab's X-ray diffraction, particle characterization, surface area, and thermal analysis facilities.

Dave Fecko and Lin Wang

Lin Wang

Focusing on bio-inspired materials, Wang translates the design principles of natural materials to synthetic materials using cutting-edge fabrication technologies.

Fabien Grisé

Grisé's research focuses on developing new technology for NASA's future space telescopes, and most specifically on a certain type of optics called gratings that are used to split light into its primary constituents. This effect is similar to the rainbow pattern that can be seen when shining light on the surface of a CD or DVD. Gratings allow astronomers to study and understand the physics at play in stars, galaxies, black hole systems, and more.

Dave Fecko and Nichole Wondering

TOWN HALL ON CHIPS AND SCIENCE ACT ENVISIONS KEY ROLE FOR PENN STATE

PENN STATE HELD a Town Hall meeting recently to discuss internal strategies around semiconductor technologies and taking on a key role in partnering with other universities and industries centered on the U.S. government's CHIPS (Creating Helpful Incentives to Produce Semiconductors) and Science Act, which was signed into law on Aug. 9, 2022. The intent of this meeting was to share Penn State's significant and spanning capabilities and expertise and facilitate internal alignment. Meetings have already taken place and will continue to occur with other university, industry, and state partners.

The CHIPS and Science Act spawned multiple funding-driven opportunities to position the U.S. as a leader in these fields, with various major new and upcoming programs sponsored by the Department of Commerce, the Department of Defense, Department of Energy, and the National Science Foundation.

To best address some of these opportunities, Penn State is creating the Mid-Atlantic Semiconductor Hub (MASH) with nine other academic partners, industry, and state governments to lead and leverage the cumulative expertise in this area.

As another example of Penn State's current involvement in semiconductor programs, the recently funded Center for Heterogeneous Integration of Micro Electronic Systems (CHIMES) was a major step in partnering to address global needs in the semiconductor space. CHIMES was announced by the Semiconductor Research Corporation (SRC)'s Joint University Microelectronics Program 2.0 (JUMP 2.0), a consortium of industrial partners in cooperation with the Defense Advanced Research Projects Agency (DARPA). The SRC funded $32.7 million to the Penn State-led Center.

Several years ago, recognizing the gaps in semiconductor technology research in the United States and the dependency on other countries, Penn State's Materials Research Institute (MRI) and Department of Electrical Engineering began prioritizing semiconductor research to better meet the needs of our national demand. Several industrial partners have also been part of this journey. Penn State has a deep commitment to interdisciplinary research as an institutional strength, including fields related to the CHIPS and Science Act such as semiconductor materials, devices, packaging, optics, thermal management/efficiencies, computation, and quantum devices. This includes a strong history in 2D materials research. All of these opportunities come with significant emphasis on workforce development, where Penn State has considerable strength to train the next generation of leaders, scientists, engineers, and manufacturers across all the manufacturing domains inherent in CHIPS needs.

"Semiconductor and chip technology have been tremendous strengths for Penn State for several years, visible in our national rankings as No. 1 and No. 2 for materials science and materials engineering," stated Lora Weiss, senior vice president for research, "This is why Penn State is an obvious choice to lead programs around the CHIPS and Science Act, and bring global recognition back home to the United States." ■

Penn State held a Town Hall on March 1 to discuss internal strategies around semiconductor technologies and Penn State taking on a key role in partnering with other universities and industry centered on the United States government's CHIPS (Creating Helpful Incentives to Produce Semiconductors) and Science Act, signed into law on Aug. 9, 2022. Credit: Materials Research Institute/Penn State

More information about MASH can be found via the QR code on the left. Questions or comments can be sent to chipsact@psu.edu.

MAURICIO TERRONES NAMED HEAD OF THE DEPARTMENT OF PHYSICS

By Sam Sholtis

MAURICIO TERRONES, EVAN PUGH UNIVERSITY PROFESSOR and Verne M. Willaman Professor of Physics, and professor of chemistry and of material science and engineering, has been named the new George A. and Margaret M. Downsbrough Head of the Department of Physics at Penn State, effective July 1. Terrones succeeds Nitin Samarth, who has served as head of the department since 2011.

Through his research, Terrones has made considerable experimental and theoretical contributions to the field of nanoscience — the physico-chemical and biological manipulation of incredibly small structures less than 100 nanometers, or less than a thousand times smaller than the width of a human hair. He studies and builds nanomaterials that exhibit novel phenomena and could potentially have industrial, biomedical and electronic applications, including carbon-based and low-dimensional materials like carbon nanotubes, graphene, and monolayers of transition metal dichalcogenides.

Terrones has co-authored over 700 papers in scientific journals, including Nature, Science,

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Mauricio Terrones, Evan Pugh University Professor and Verne M. Willaman Professor of Physics, and professor of chemistry and of material science and engineering

Nature Nanotechnology, Nature Materials, Physical Review Letters, Nano Letters, Proceedings of the National Academy of Sciences, and Applied Physics Letters. His research articles have been cited more than 80,000 times worldwide, and he has been named a "Highly Cited Researcher" by Clarivate for the years 2017 through 2022. Terrones helped create Penn State's Center for 2-Dimensional and Layered Materials and has been the center's director since 2013. He also is director of the NSF-IUCRC Center for Atomically Thin Multifunctional Coatings (ATOMIC) at Penn State and editor-in-chief of the highly-cited journal Carbon.

Terrones has been honored in the past with the Chair of Excellence from Universidad Carlos III de Madrid (UC3M) and Banco Santander in 2018; the Faculty Scholar Medal for Outstanding Achievement in the Physical Sciences from Penn State in 2016; the Somiya Award for International Collaboration in Materials Research from the International Union of Materials Research Societies in 2009; the Japan Carbon Award for Innovative Research from the Japan Carbon Society TANSO in 2008; the Scopus Prize from Elsevier in 2007; the Fernando Alba Medal from the National Autonomous University of Mexico in 2007; The World Academy of Sciences (TWAS) Prize in Engineering in 2006; the Javed Husain Prize and the Albert Einstein Medal from the United Nations Educational, Scientific and Cultural Organization (UNESCO) in 2001; and the Mexican National Prize for Chemistry in 2000. He is an elected Fellow of the American Association for the Advancement of Science, the Royal Society of Chemistry (UK), the American Physical Society, the Academy of Sciences for the Developing World, and the Mexican Academy of Sciences.

Terrones was named Verne M. Willaman Professor of Physics at Penn State in 2019 and an Evan Pugh Professor, the highest honor that Penn State bestows on a faculty member, in 2022. Prior to joining the Penn State faculty in 2011, Terrones was a professor at the Universidad Carlos III in Spain, Distinguished Professor at Shinshu University in Japan and Professor at the Instituto Potosino de Investigación Científica y Tecnológica (IPICYT) in San Luis Potosí, Mexico. He was an Alexander von Humboldt Fellow at the Max-Planck-Institut für Metallforschung in Germany in 1999, and a postdoctoral research fellow at the University of Sussex from 1997 to 1999. Terrones obtained a doctoral degree in chemical physics at the University of Sussex under the supervision of Nobel Laureate Harold W. Kroto in 1997 and a bachelor's degree in engineering physics with first class honors at Universidad Iberoamericana in Mexico in 1992. ■

Randall McEntaffer, head of Penn State's Department of Astronomy and Astrophysics, makes adjustments to the flight electronics and power supply of the X-ray spectrometer that he and his team built for a September launch with NASA. Credit: Patrick Mansell/Penn State Creative Commons

Penn State's $1.034B in research expenditures has broad, wide-ranging impact

PENN STATE REACHED a record $1.034 billion in research expenditures during fiscal year 2021-22, an overall 4.1% increase from the previous year. The funding, which comes from federal and state agencies, industry sponsors, private donors, the University, and other sources, advances research innovations and enables Penn State faculty and students to push the boundaries of discovery, bringing experiences into the classrooms, and offering a world-class education to undergraduate and graduate students.

"This marks a banner year in the trajectory of research at Penn State," said Penn State President Neeli Bendapudi. "We are proud that funders view Penn State as a pillar of high-quality research and education. Their significant investments in the University are a testament to the abilities of our faculty, staff, and students to create knowledge, innovations, and technologies that help advance our land-grant mission."

The total figure, $1.034 billion, places Penn State among a select group of research universities nationally and reflects the interdisciplinary strength built over more than three decades. Penn State continues to rank in the top 25 academic institutions by expenditures with 12 disciplines ranked in the top 10. Only three other universities in the nation have more top-10 ranked disciplines.

Funding from federal agencies comprised the majority of Penn State's research expenditures, totaling a record $663.7 million in fiscal year 2022, a $53.7 million increase from the previous year. Awards contributing to this include:

- $25 million from the National Institutes of Health to improve access to clinical trials and new medical and behavioral treatments and interventions for residents of Pennsylvania.

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- $20 million from the National Science Foundation to develop high-performance materials that can be used to create flexible electronics, among other novel applications.

- $17 million from the Department of Energy to study climate change resilience in cities.

Nearly 27% of overall funding is attributed to the Applied Research Laboratory, a Department of Defense-designated university affiliated research center, dedicated to conducting research that helps secure our nation while simultaneously preparing students for careers in national security.

Federal funding also provided significant support for graduate and undergraduate students. For example, in 2020-21, external grants and contracts provided $65.9 million in graduate student stipend support.

Expenditures for fiscal year 2022 also included $26 million in industry sponsorships from several hundred companies. These industry partnerships are driving economic development, training the workforce of the future, and facilitating technology transfer in a variety of public-private partnerships.

For more information about research at Penn State, go to research.psu.edu. ■

Penn State team awarded National Science Foundation I-Corps grant

By Jamie Oberdick

THE BIGGEST QUESTION an entrepreneur faces is a simple one: Are there enough potential customers to turn my big idea into a business? A trio of Penn State researchers were selected recently for the National Science Foundation's (NSF) National I-Corps Program to find an answer for their own big idea.

The three researchers are Saptarshi Das, associate professor of engineering science and mechanics; Sarbashis Das, doctoral candidate in electrical engineering; and Harikrishnan Ravichandran, doctoral candidate in engineering science and mechanics. Their big idea is to offer a foundry service for manufacturing sensors and integrated circuits made of two-dimensional (2D) materials for use in a variety of industries including Internet of Things (IoT) applications, food processing, pharmaceutical and various defense needs.

This company is envisioned to be a fabrication facility that would create custom devices based on specific customer needs. Their initial research suggests a possibility that there may be a demand for such sensors in industries such as food processing, medical devices, and automotive. If they develop a company, they can become another industry partner of the Materials Research Institute (MRI) and use the facilities in the Millennium Science Complex to manufacture and characterize the products like the other partners.

NSF I-Corps is a comprehensive entrepreneurial training program designed to transform research ideas and findings

From left to right, Sarbashis Das, doctoral candidate in electrical engineering; Saptarshi Das, associate professor of engineering science and mechanics; and Ravichandran Harikrishnan, doctoral candidate in engineering science and mechanics in their lab in Penn State's Millennium Science Complex. Credit: Jamie Oberdick/Penn State

into products that positively impact society. The team first participated in the regional Mid-Atlantic NSF I-Corps, which inspired them to apply for the national program. They were accepted and received a $50,000 grant as part of joining the program.

"The $50,000 cannot be used for any direct research purposes, instead it will be used for customer discovery," Sarbashis Das said. "So, we will find out who can be our future customers and learn if we have enough customers to start a sustainable business, which is the ultimate question for any entrepreneur."

To do this, the team will conduct 100 interviews with potential customers over about six weeks. These interviews will be with representatives from a wide variety of different companies. Saptarshi Das noted that they may discover that their preconceived notions about what the industry wants could be completely wrong. So, doing the interviews could give them an idea that what their research is focused on might not be what potential customers are looking for.

"For example, we have always thought that sensor costs were a very important thing, but from the customers we have already spoken with, we have learned that the cost is not always important," he said. "Some of the industries are willing to pay the price if the sensors work well and prevent problems. That was a revelation because when we author papers, we always stress that our sensors are low cost, and low power, but that is not always what the customers will be looking for. They want to make sure that it solves their specific problems."

One potential issue their sensors could solve is finding contaminants in food processing.

"We found that our sensors, which are graphene based, can be used for identifying undesired species in a liquid solution, which is of obvious interest to the food processing industry," Saptarshi Das said. "You are offering better sensors to prevent unwanted contaminants or species in your food product. That is a direct benefit for the society." ■

3D printing of medical devices focus of $2 million NSF grant

By Mary Fetzer

ADDITIVE MANUFACTURING TECHNOLOGY, also known as 3D printing, provides the opportunity to create customized medical devices. However, the capabilities to design and print the smart, flexible materials this type of equipment requires remain lacking, according to researchers at Penn State and The University of Texas at Austin.

Those researchers are working to change that. A $2 million grant from the National Science Foundation (NSF)'s Leading Engineering for America's Prosperity, Health and Infrastructure (LEAP-HI) program will pave the way for the researchers to tackle the challenge of designing and 3D printing smart devices using multiple materials.

"The project allows us to collaborate at the exciting intersection of advanced manufacturing, soft materials, and adaptive structures," said project co-lead Mary Frecker, professor of mechanical engineering and of biomedical engineering, head of Department of Mechanical Engineering and Reiss Chair of Engineering at Penn State. "The results will benefit patients by enabling shape change in medical devices."

The researchers will work with Pennsylvania-based medical device company Actuated Medical Inc., which is led by Maureen Mulvihill, president and chief executive officer, who earned a doctorate of materials science and engineering from Penn State. Together, they plan to use 3D printing techniques to design pediatric ventilation masks and other medical devices that can be customized into different shapes during use.

They aim to pioneer new ways to print and actuate these multi-material devices, along with new methods for designing them, that take the capabilities of the additive manufacturing process into account and avoid expensive, iterative testing and refinement.

Leading the project with Frecker — who is also the director of the Penn State Center for Biodevices — and Seepersad are Penn State's Zoubeida Ounaies, director of the Convergence Center for Living Multifunctional Materials Systems, acting director of the Materials Research Institute, and professor of mechanical engineering; and Lorraine Dowler, professor of geography and of women's, gender, and sexuality studies.

Though 3D printing has been around for several decades, few researchers have cracked the code on how to use additive manufacturing to create smart, multi-material objects and devices. The researchers envision printing smart devices that can change shape to accommodate shifting requirements, fabricating them in a single additive manufacturing process

Project co-leads include Zoubeida Ounaies, director of the Convergence Center for Living Multifunctional Materials Systems, acting director of the Materials Research Institute and professor of mechanical engineering; Mary Frecker, professor of mechanical engineering and of biomedical engineering, head of Department of Mechanical Engineering and Reiss Chair of Engineering; and Lorraine Dowler, professor of geography and of women's, gender and sexuality studies. Credit: Jeff Xu/Penn State

and customizing each device with a computationally efficient approach that ensures manufacturability.

In addition to the technical goals of the project the researchers will chronicle how they think, collaborate and lead within their institutional structures to get a better understanding of diversity in engineering teams and projects.

"There have been numerous research studies that argue that diverse teams, both inherent — e.g., race, gender, sexuality — and acquired — e.g., education, geography, cultural background — lead to innovation," said Dowler, who will document how diverse leadership leads to diverse results. "However, it is rare to have an opportunity to conduct a multi-year study that observes the day-to-day decision-making processes of diverse leadership and how that leads to both product innovation and job satisfaction for the entire team. The leadership team for this prestigious grant is all women, which, if not the first, is certainly rare in mechanical engineering." ■

Editor's note: A version of this press release appeared on The University of Texas at Austin's news site.

NSF grant expands materials science research at Penn State Behrend

Beth Last, the research core facilities coordinator at Penn State Behrend, is the co-principal investigator for a $385,000 National Science Foundation grant at the college. Credit: Penn State Behrend/Penn State

ERIE, PA. — A $385,000 grant from the National Science Foundation will fund the purchase of an Instron drop tower impact-testing system at Penn State Behrend, where faculty members are developing new approaches to polymer recycling and the formulation of new composites.

At least 10 faculty members will use the system to advance their research, which includes automotive and aerospace partnerships. Another will use it to test new polymers for ski boots and bindings.

The Instron system will expand the materials research capabilities at Behrend, where grant funding and industry partnerships fueled $8.3 million in research expenditures in 2021.

"This takes us into a whole new kind of materials science," said Greg Dillon, chair of the Polymer Engineering and Science program at Behrend and the principal investigator for the NSF grant. "It allows us to delve very deeply into fracture mechanics: how materials and structures fail under high energy."

Drop towers are used to determine how materials break. The drop mechanism, or tup, is fired like an arrow into a plastic, metal, ceramic or gel. The Instron tup drops at a rate of 78 feet per second.

"It's a lot like a crossbow," said Alicyn Rhoades, the interim associate dean for research and graduate studies at Behrend. She and Dillon wrote the original application for the NSF grant.

For a previous study, during a sabbatical, Rhoades used a drop tower owned by a corporate partner. The tup on that machine had been customized for the company's product, however, so it was not practical to collaborate on the machine for University projects.

Rhoades and Dillon began the process of acquiring a drop tower at Behrend. The Instron system they selected will include a variety of tups — round, flat, and conical — that can be changed based on an individual researcher's needs. The conditioning chamber can be heated or cooled to test how a material responds at different temperatures, from a high of 302 degrees Fahrenheit to a low of -94 degrees.

"Any time you test, you want to do so in conditions that are as close to the actual product environment as possible," said Beth Last, the research core facilities coordinator at Behrend and the co-principal investigator for the grant.

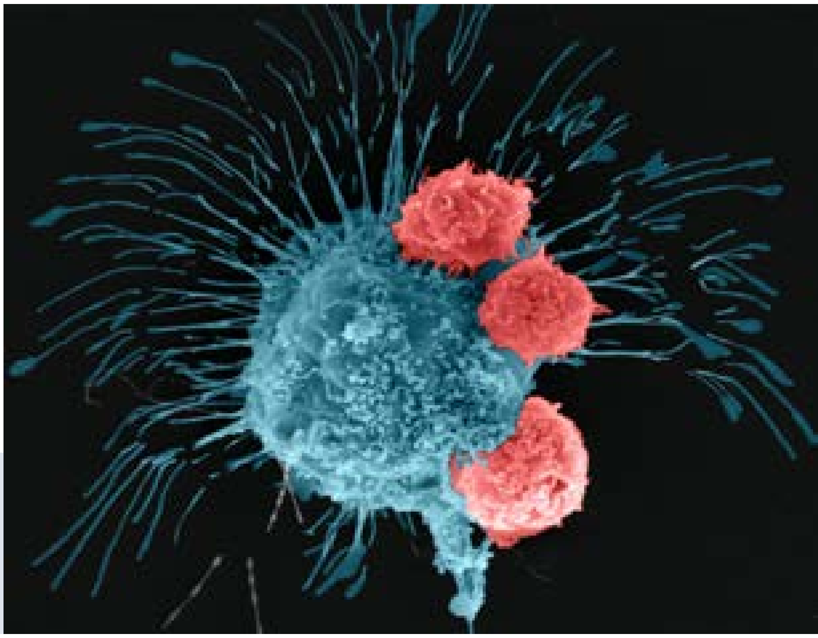
A high-speed camera on the Instron system will allow Behrend researchers to analyze the entire process. The camera, which can be set to different magnifications, can record 900,000 frames every second.

Like a Harold Edgerton photo — the bullet piercing the apple, or the splash of milk forming a perfect white crown — those images essentially stop time: Researchers can see the exact moment a crack or fracture forms. Then, a few frames ahead, they can watch it spread.

"You can see what's happening within the material," Dillon said. "Is it bending? Does it deform? Does it in any way resist the impact? Once you know that, you can engineer materials that better absorb that energy." ■

research SNAPSHOTS

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



A scanning electron microscopy image shows a breast cancer cell (cyan) being attacked by T cells (red), which were engineered to recognize the cancer cells. Credit: Madhuri Dey, courtesy of the Ozbolat Lab/Penn State

Researchers 3D bioprint breast cancer tumors, treat them in groundbreaking study

By Adrienne Berard

RESEARCHERS AT PENN State have successfully 3D bioprinted breast cancer tumors and treated them in a breakthrough study to better understand the disease that is one of the leading causes of mortality worldwide.

A scientific first, the achievement lays the foundation for precision fabrication of tumor models. The advancement will enable future study and development of anti-cancer therapies without the use of "in vivo" — or "in animal" — experimentation.

"This will help us understand how human immune cells interact with solid tumors," said Ibrahim Ozbolat, professor of engineering science and mechanics, biomedical engineering, and neurosurgery at Penn State and the senior author of the study. "We've developed a tool that serves as a clinical test platform to safety and accurately evaluate experimental therapies. It is also a research platform for immunologists and biologists to understand how the tumor grows, how it interacts with human cells, and how it metastasizes and spreads in the body."

Ozbolat's lab specializes in 3D printing to create a range of tissues for use in human health. Two journal articles about the lab's work using 3D bioprinting to help in the study of breast cancer were recently published in Advanced Functional Materials and Biofabrication.

The researchers used a relatively new technique called aspiration-assisted bioprinting to precisely locate tumors in three dimensions and create the tissue. The researchers then formed the tissue into a multi-scale vascularized breast tumor model with blood vessels, which they discovered responded to chemotherapy and cell-based immunotherapeutics.

The team first validated the accuracy of its tumor model by treating it with doxorubicin, an anthracycline-based chemotherapeutic drug commonly used for treating breast cancer. Finding the bioprinted tumor responded to chemotherapy, the researchers went on to test a cell-based immunotherapeutic treatment on the tumor in collaboration with Dr. Derya Unutmaz, an immunologist at Jackson Laboratory.

The researchers used human CAR-T cells that were engineered via gene editing to recognize and fight an aggressive form of breast cancer cells. After 72 hours of circulating the edited CAR-T cells through the tumor, the researchers found that the cells within the bioprinted tumor had generated a positive immune response and were fighting off the cancer cells.

"Our model is made from human cells, but what we make is a very simplified version of the human body," Ozbolat said. "There are many details that exist in the native microenvironment that we aren't able to replicate, or even consider replicating. We are aiming for simplicity within complexity. We want to have a fundamental understanding of how these systems work — and we need the growth process to be streamlined, because we don't have time to wait for tumors to grow at their natural pace."

Ozbolat and his colleagues are now working with tumors removed from actual breast cancer patients. The researchers will apply immunotherapeutics to patient-derived tumors to see how they respond.

"This is an important step in understanding the intricacies of the disease, which is essential if we are going to develop novel therapeutics and targeted therapies against cancer," Ozbolat said. ■

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To read the full story:

Engineers improve electrochemical sensing by incorporating machine learning

By Mary Fetzer

COMBINING MACHINE LEARNING with multimodal electrochemical sensing can significantly improve the analytical performance of biosensors, according to new findings from a Penn State research team. These improvements may benefit noninvasive health monitoring.

The researchers developed a novel analytical platform that enabled them to selectively measure multiple biomolecules using a single sensor, saving space and reducing complexity as compared to the usual route of using multi-sensor systems. In particular, they showed that their sensor can simultaneously detect small quantities of uric acid and tyrosine — two important biomarkers associated with kidney and cardiovascular diseases, diabetes, metabolic disorders, and neuropsychiatric and eating disorders — in sweat and saliva, making the developed method suitable for personalized health monitoring and intervention.

Many biomarkers have similar molecular structures or overlapping electrochemical signatures, making it difficult to detect them simultaneously. Leveraging machine learning for measuring multiple biomarkers can improve the accuracy and reliability of diagnostics and as a result improve patient outcomes, according to the researchers. Further, sensing using the same device saves resources and biological sample volumes needed for tests, which is critical with clinical samples with scarce amounts.

Aida Ebrahimi, Thomas and Sheila Roell Early Career Assistant Professor of Electrical Engineering and assistant professor of biomedical engineering, and Vinay Kammarchedu, 2022-23 Milton and Albertha Langdon Memorial Graduate Fellowship in Electrical Engineering, developed a new approach to improve the performance of electrochemical biosensors by combining machine learning with multimodal measurement. Credit: Kate Myers/Penn State

"We developed a new approach to improve the performance of electrochemical biosensors by combining machine learning with multimodal measurement," said Aida Ebrahimi, Thomas and Sheila Roell Early Career Assistant Professor of Electrical Engineering and assistant professor of biomedical engineering. "Using our optimized machine learning architecture, we could detect biomolecules in amounts 100 times lower than what conventional sensing methods can do."

The researchers' methodology features a hardware/software system that enables them to automatically gather and process information based on a machine learning model that is trained to identify biomolecules in biological fluids such as saliva and sweat, which are common choices for noninvasive health monitoring.

"The machine learning-powered electrochemical diagnostic approach presented in this paper may find broader application in multiplexed biochemical sensing," said Vinay Kammarchedu, 2022-23 Milton and Albertha Langdon Memorial Graduate Fellow in Electrical Engineering at Penn State and first author on the paper.

In their ongoing work, the researchers are applying this approach on such neurochemicals, which are difficult to detect due to similarities in their molecular structure and overlapping electrochemical signatures.

Beyond the specific results with the uric acid and tyrosine, the researchers are excited about the potential and versatility of the methodology.

"It is a new way of designing electrochemical diagnostic methods that may be applied to a variety of applications beyond biomedical systems," Ebrahimi said.

Combined with innovations in material and device engineering for sensor development, the researchers' analytical method may provide opportunities in pharmaceuticals, life science research, food screening, detection of environmental toxins and biodefense, where accurate and multiplexed testing or in-line monitoring is needed.

In the researchers' current prototype stage, the hardware is benchtop sized. They are working to make a smaller system that can be implemented for more than just health monitoring.

"Ultimately, we envision a handheld and field-deployable device that will be easier to use and more readily available than the current practices used in laboratory or clinical settings," Kammarchedu said. ■

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2D material may enable ultra-sharp cellphone photos in low light

By Jamie Oberdick

A NEW TYPE OF active pixel sensor that uses a novel two-dimensional material may both enable ultra-sharp cellphone photos and create a new class of extremely energy-efficient Internet of Things (IoT) sensors, according to a team of Penn State researchers.

"When people are looking for a new phone, what are the specs that they are looking for?" said Saptarshi Das, associate professor of engineering science and mechanics and lead author of the study published Nov. 17 in Nature Materials. "Quite often, they are looking for a good camera, and what does a good camera mean to most people? Sharp photos with high resolution."

Most people just snap a photo of a friend, a family gathering, or a sporting event, and never think about what happens "behind the scenes" inside the phone when one snaps a picture.

"When you take an image, many of the cameras have some kind of processing that goes on in the phone, and in fact, this sometimes makes the photo look even better than what you are seeing with your eyes," Das said. "These next generation of phone cameras integrate image capture with image processing to make this possible, and that was not possible with older generations of cameras."

The innovation in materials outlined in the study revolves around how they added in-sensor processing to active pixel sensors to reduce their energy use. So, they turned to a novel 2D material, which is a class of materials only one or a few atoms thick, molybdenum disulfide. It is also a semiconductor and sensitive to light, which makes it ideal as a potential material to explore for low-energy in-sensor processing of images.

"We found that molybdenum disulfide has very good photosensitive response," said Darsith Jayachandran, graduate research assistant in engineering and mechanics and co-first author of the study. "From there, we tested it for the other properties we were looking for."

New method can scale, simplify manufacture of stretchy semiconductors

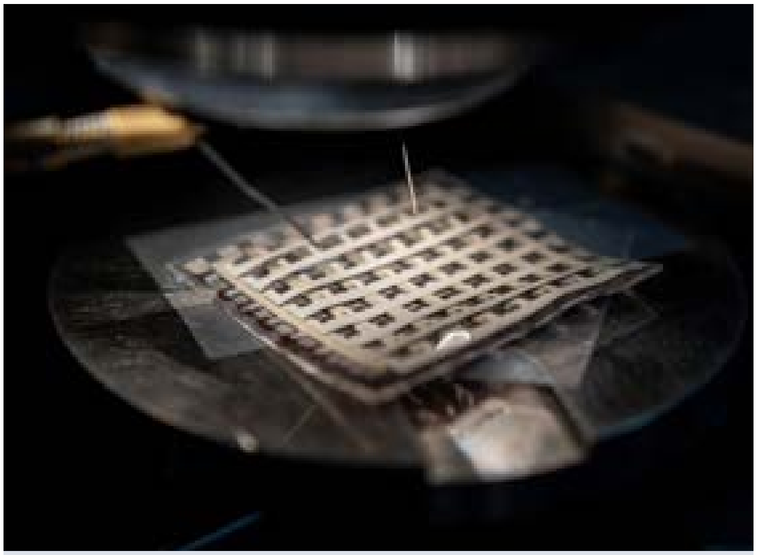
By Mariah R. Lucas

SOFT, ELASTIC SEMICONDUCTORS and circuits could advance wearable medical devices and other emerging technologies, but the high-performance electronics are difficult and expensive to manufacture. A Penn State-led research team plans to make the process easier and cheaper with a new manufacturing method.

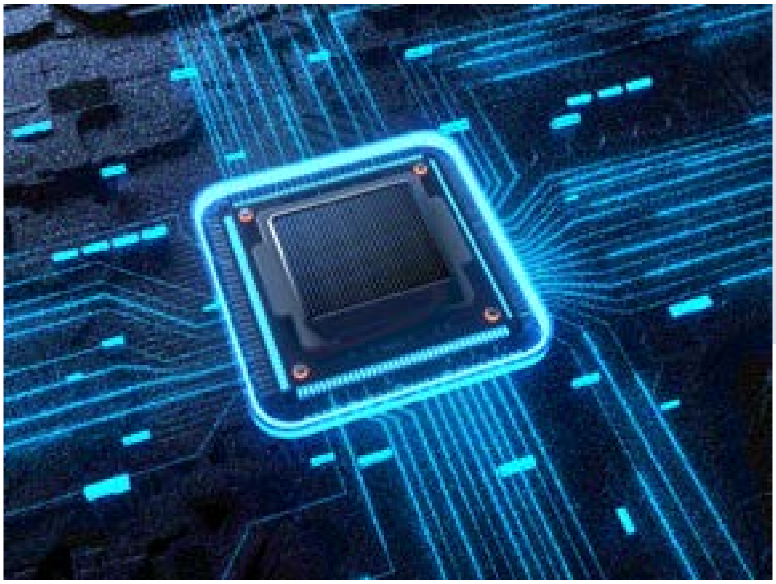
They published their approach Nov. 28 in Nature Electronics.

Known as the lateral phase separation induced micromesh (LPSM) strategy, the process involves mixing a semiconductor and an elastomer — or rubber — and spin coating the liquid mixture precursors to fabricate rubbery semiconductor thin films. The spin coated film automatically triggers a mechanism called lateral phase separation, which generates micromesh structures within seconds.

The micromesh materials, which resemble a basket weave, are integral for allowing for mechanical stretch, according to Cunjiang



Penn State researchers developed stretchy transistors, like the one pictured, using a new method known as the lateral phase separation induced micromesh strategy. The micromesh materials, which resemble a basket weave, are integral for allowing for mechanical stretch. Credit: Jeff Xu



New pixel sensors based on monolayer molybdenum disulfide offer better imaging capabilities. Credit: Elizabeth Floresgomez Murray/Penn State

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These properties included sensitivity to low light, which is important for the dynamic range of the sensor. The dynamic range refers to the ability to "see" objects in both low light such as moonlight and bright light such as sunlight. The human eye can see stars at night better than most cameras due to having superior dynamic range.

Molybdenum disulfide also demonstrated strong signal conversion, charge-to-voltage conversion and data transmission capabilities. This makes the material an ideal candidate to enable an active pixel sensor that can do both light sensing and in-sensor image processing.

The dynamic range and image processing would enable users to take sharp photos in a variety of adverse conditions for photography, according to Das.

"For example, you could take clearer photos of friends outside at night or on a rainy or foggy day," Das said. "The camera could do denoising to clear up the fog and the dynamic range would enable say a night photo of a friend with stars in the background." ■

Yu, Dorothy Quiggle Career Development Associate Professor of Engineering Science and Mechanics and associate professor of biomedical engineering and of materials science and engineering.

"The LPSM films used to create the stretchy semiconductors promise simultaneous efficient charge transport and mechanical stretchability," Yu said.

Researchers used the LPSM method to create both p-type and n-type semiconductors, whose majority charge carriers are holes and electrons, respectively. Using both semiconductor types, according to Yu, researchers created soft electronic devices such as transistors, inverters and photodetectors that can stretch to a large extent while maintaining functionality. In addition, the researchers created a rubbery bioelectronic device known as an epicardial patch and implanted it in a rodent.

"As the rat's heart expanded and contracted with its heartbeat, the entirely rubber-based epicardial patch also moved with it," Yu said. "We recorded multiple channels of electrophysiology readings simultaneously with the patch. Recording at multiple sites of the heart is important to identify cardiac problems such as arrhythmia."

Going forward, researchers hope to further optimize the LPSM process and to investigate the detailed properties of the semiconductor materials, according to Yu. They also plan to employ the LPSM semiconducting thin film in various high-performance integrated electronics and functional systems.

In addition to Yu, the co-authors include Ying-Shi Guan, Southeast University, China and the University of Houston; Faheem Ershad, Department of Biomedical Engineering, Penn State and the University of Houston; Zhoulyu Rao and Yuntao Lu, Department of Engineering Science and Mechanics, Penn State and the University of Houston; Zhifan Ke and Jianguo Mei, Purdue University; Ernesto Curty da Costa, Qian Xiang, Peter Vanderslice, and Camila Hochman-Mendez, Texas Heart Institute; Xu Wang, the University of Houston.

The animal research procedures were approved by the Texas Heart Institute's Institutional Animal Care and Use Committee.

The National Science Foundation, the National Institutes of Health, and the Office of Naval Research supported this work. ■

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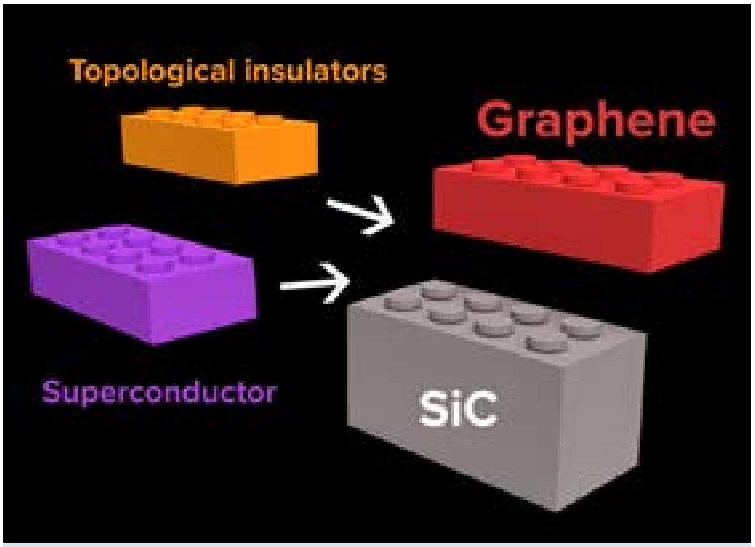
New material may offer key to solving quantum computing issue

By Jamie Oberdick

A NEW FORM OF a heterostructure of layered two-dimensional (2D) materials may enable quantum computing to overcome key barriers to its widespread application, according to an international team of researchers.

The researchers were led by a team that is part of the Penn State Center for Nanoscale Science (CNS), one of 19 Materials Research Science and Engineering Centers (MRSEC) in the United States funded by the National Science Foundation. Their work was published Feb. 13 in Nature Materials.

A regular computer consists of billions of transistors, known as bits, and is governed by binary code ("0" = off and "1" = on). A quantum bit, also known as a qubit, is based on quantum mechanics and can be both a "0" and a "1" at the same time. This is known as superposition and can enable quantum computers to be more powerful than regular, classical computers.



The formation of heterostructure of a layered two-dimensional material envisioned as Lego blocks locking together. Image by Elizabeth Floresgomez Murray

Researchers use water treatment method to capture acids from agricultural waste

By Mariah R. Lucas

UNIVERSITY PARK, PA. — Bound for the landfill, agricultural waste contains carbon sources that can be used to produce high-value compounds, such as p-coumaric acid, which is used in manufacturing pharmaceuticals. Electrodeionization, a separation method that uses ion-exchange membranes, is one way to capture the acids and other useful components. However, to capture large quantities at scale, improvements to the method must be made.

A Penn State-led research team has invented a new class of ion-exchange membrane wafer assemblies that significantly improves electrodeionizaton's ability to capture p-coumaric acid from liquid mixtures while using less energy and saving money. The researchers published their results in ACS Sustainable Chemical Engineering. Their article also was selected for the journal's Jan. 23 cover.

First commercialized to purify water, electrodeionization has been used to capture valuable components from waste streams in recent years. In the process, a liquid mixture stream is fed through a stack of several ion-exchange membranes and resin wafers, which resemble a sponge and are held together with a polymer adhesive. When electricity is applied, the ions in the liquid move through the stack, and p-coumaric acid separates into a concentrated process stream, where it can then be collected.

"To improve the process, we had to improve upon the resin wafer," said corresponding author Chris Arges, Penn State associate professor of chemical engineering. "Previously, the membranes would sandwich the resin wafer sponge with a polyethylene adhesive, which is currently used in industry as resin 'glue,' but this led to poor contact between the membrane and resin wafer. We substituted the polyethylene with imidazolium ionomer, a type of polymer, and glued an imidazolium membrane on top of the resin wafer."

By gluing the membrane to the wafer, the researchers reduced the amount of membrane needed by 30%, reducing the cost of the electrodeionization unit. The new design also reduced the interfacial

"IBM, Google, and others are trying to make and scale up quantum computers based upon superconducting qubits," said Jun Zhu, Penn State professor of physics and corresponding author of the study. "How to minimize the negative effect of a classical environment, which causes error in the operation of a quantum computer, is a key problem in quantum computing."

A solution for this problem may be found in an exotic version of a qubit known as a topological qubit.

"Qubits based on topological superconductors are expected to be protected by the topological aspect of the superconductivity and therefore more robust again the destructive effects of the environment," Zhu said.

There is currently a lot of focus on topological quantum computing, according to Cequn Li, graduate student in physics and first author of the study.

"Quantum computing is a very hot topic and people are thinking about how to build a quantum computer with less error in the computation," Li said. "A topological quantum computer is an appealing way to do that. But a key to topological quantum computing is developing the right materials for it."

The study's researchers have taken a step in this direction by developing a type of layered material called a heterostructure. The heterostructure in the study consists of a layer of a topological insulator material, bismuth antimony telluride or (Bi,Sb)2Te3, and a superconducting material layer, gallium.

However, such a topological insulator/superconductor heterostructure is difficult to create.

"It's not easy usually because different materials have different lattice structures," Li said. "Also, if you put two materials together, they may react with one another chemically and you end up with a messy interface."

Therefore, the researchers are using a synthesis technique known as confinement heteroepitaxy, which is being explored at MRSEC. This involves inserting a layer of epitaxial graphene, which is a sheet of carbon atoms of one or two atoms thick, between the gallium layer and the $(Bi, Sb)_2Te_3$ layer. Li notes this enables the layers to interface and combine, like snapping Lego blocks together.

In addition, the researchers demonstrated that this technique is scalable at the wafer level, which would make it an attractive option for future quantum computing.

This research was a combined effort of the CNS's IRG1 – 2D Polar Metals and Heterostructures team, led by Zhu and Joshua Robinson, professor of materials science and engineering at Penn State. Other faculty involved in the research include Cui-Zu Chang, Henry W. Knerr Early Career Professor and associate professor of physics, and Danielle Reifsnyder Hickey, assistant professor of chemistry and materials science and engineering. ■

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resistance between the membrane and the wafer, as the same membrane and binder chemistries were glued together rather than sitting on top and below the sponge with air gaps. Reducing the resistance led to an increased rate of capturing p-coumaric acid, allowing researchers to use a smaller unit.

Kumar, associate professor of chemistry at Louisiana State University, found the imidazolium increases the solubility of the p-coumaric acid and spurs faster diffusion within the material.

"Multiplied together, solubility and diffusion equal permeability, or how fast we remove the acid as it travels across the membrane resin wafer network into the concentrate compartment," Arges said.

Arges compared permeability to the rate of travelers going through an airport security line. As more security checkpoints are added, more people can move through the line, increasing the line's permeability.

"The imidazolium membrane resin wafer assembly promotes the flow of p-coumaric acid through the membrane, which is a problem when other materials, like polyethylene, are used," Arges said.

When benchmarked against the current resin wafer configuration, the new membrane configuration and materials result in a sevenfold increase in p-courmaric acid capture while using 70% less energy, accor+ding to researchers. The new assemblies also decrease the amount of membrane used in the process, resulting in significant cost savings. ■

A Penn State-led research team has invented a new class of ion-exchange membrane wafer assemblies that significantly improves electrodeionizaton's ability to capture p-coumaric acid from liquid mixtures. Credit: Jeff Xu/Penn State

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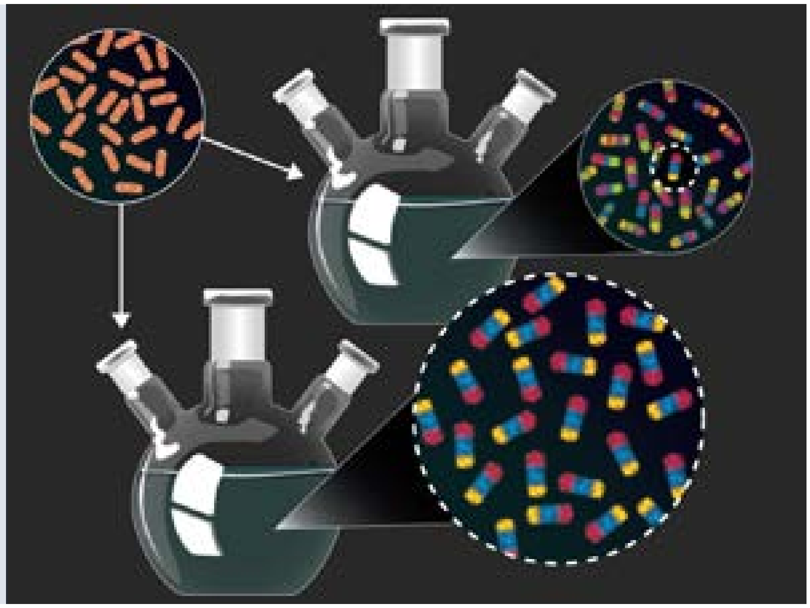
research SNAPSHOTS



Researchers start with simple rod-shaped nanoparticles (top left) composed of a single material, copper sulfide. In purposely unoptimized experiments (top), the researchers produced and characterized hundreds of nanoparticles which combine many different materials in various arrangements. They then used new guidelines derived from the first set of experiments to rationally produce one of the nanoparticles in high yield (bottom). Credit: Dani Zemba and the Schaak Laboratory/Penn State

Unconventional experiments produce new nanoscale particles with big potential

By Sam Sholtis

HUNDREDS OF NEW nanoparticles with previously unknown features have been produced using an innovative experimental approach.

Chemists usually make materials by finding the best conditions to target a single product. A research team at Penn State flipped this approach on its head by purposely using unoptimized conditions to produce many products at once. This approach allowed them to discover novel nanoparticles, which combine many different materials in various arrangements. They then analyzed these nanoparticles to develop new guidelines that allowed them to make high-yield samples of the most interesting types of new nanoparticles.

"There are a certain number of rules that we and others have developed in this field that allow us to make a lot of different kinds of nanoparticles," said Raymond Schaak, DuPont Professor of Materials Chemistry at Penn State and the leader of the research team. "We can also predict, especially with the help of computers, tens of thousands of different nanoparticles that could be really interesting to study, but we have no clue how to make most of them. We need new rules that allow us to make nanoparticles with new properties, new functions, or new applications, and that allow us to better match the speed at which they can be predicted."

The current set of rules, or design guidelines, available to researchers limits the variety of nanoparticles that they can produce, so the researchers set up experiments under unoptimized and previously unexplored conditions to see if they could make new types of particles that hadn't previously been discovered.

The researchers start with relatively simple rod-shaped nanoparticles composed of a single material, copper sulfide, which contains charged atoms ("cations") of copper. They can then replace some or all of the copper in the particles with other metals using a process called "cation exchange." The arrangement of the metals in the particles and the interfaces between them determine the properties of the particles. Generally, this process is done one metal at a time using experimental conditions optimized to precisely control the cation exchange reaction. Here, in one experiment, the researchers added four different metal cations at the same time under conditions that were not optimized for any particular metal cation exchange. They then painstakingly characterized the resulting particles using electron microscopy and X-ray diffraction.

The team then performed the experiment using slightly altered variables, changing the temperature of the reaction or the relative amount and variety of metal cations. By doing this, they produced even more complex nanoparticles and eventually were able to figure out the new rules that explained how the new types of nanoparticles had formed.

Finally, the team chose one of the new products and used the new design guidelines to efficiently produce it in larger quantities.

"Eventually, this approach could be used to screen for new particles with specific properties, but currently we are focusing on learning as much as we can about what all is possible to make," said Schaak. "We've demonstrated that this exploratory approach can indeed help us to identify these 'new rules' and then use them to rationally produce new complex nanoparticles in high yield." ■

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Researchers uncover mechanisms to easily dry, redisperse cellulose nanocrystals

By Maria R. Lucas

CELLULOSE NANOCRYSTALS — bio-based nanomaterials derived from natural resources such as plant cellulose — are valuable for their use in water treatment, packaging, tissue engineering, electronics, antibacterial coatings, and much more. Though the materials provide a sustainable alternative to non-bio-based materials, transporting them in liquid taxes industrial infrastructures and leads to environmental impacts.

A team of Penn State chemical engineering researchers studied the mechanisms of drying the nanocrystals and proposed nanotechnology to render the nanocrystals highly redispersible in aqueous mediums, while retaining their full functionality, to make them easier to store and transport. They published their results in the journal Biomacromolecules. The work was featured on the Jan. 17 journal cover.

"We looked at how we could take hairy nanocrystals, dry them in ovens, and redisperse them in solutions containing different ions," said co-first author Breanna Huntington, current chemical engineering doctoral student at the University of Delaware and former member of the Sheikhi Research Group while an undergraduate student at Penn State. "We then compared their functionality to conventional, non-hairy cellulose nanocrystals."

The nanocrystals have negatively charged cellulose chains at their ends, known as hairs. When rehydrated, the hairs repel each other and separate, dispersing again through a liquid, as a result of electrosteric repulsion — a term meaning charge-driven, or electrostatic, and free-volume dependent, or steric.

"The hairy ends of the nanocrystals are nanoengineered to be negatively charged and repel each other when placed in an aqueous medium," said corresponding author Amir Sheikhi, Penn State assistant professor of chemical engineering and of biomedical engineering. "To have maximum function, the nanocrystals must be separate, individual particles, not chained together as they are when they are dry."

After the hairy particles were redispersed, researchers tested them and measured their size and surface properties and found their characteristics and performance were the same as those that had never been dried. They also found the particles could perform well and maintain their stability in a variety of liquid mixtures of different salinities and pH levels.

"The hairy nanocrystals can become redispersed even at high salt concentrations, which is convenient, as they remain functional in harsh media and may be used in a broad range of applications," said co-first author Mica Pitcher, Penn State doctoral student in chemistry, supervised by Sheikhi. "This work may pave the way for sustainable and large-scale processing of nanocelluloses without using additive or energy-intensive methods."

The Penn State College of Engineering Summer Research Experiences for Undergraduates program and the NASA Pennsylvania Space Grant Consortium graduate fellowship program supported this work. ■

First author Breanna Huntington (left), current chemical engineering graduate student at the University of Delaware and former member of the Sheikhi Research Group, readies a sample of hairy cellulose nanocrystals to dry in an oven. Co-authors Mica Pitcher (center), Penn State doctoral student in chemical engineering, and Amir Sheikhi (left), Penn State assistant professor of chemical engineering, look on. Credit: Jeff Xu/Penn State

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MASH Partner Spotlight: Boston University

ANY SUCCESSFUL PARTNERSHIP relies on three things: leveraging each partner's expertise, creating an environment that nurtures collaboration, and last but not least, listening to each other. This is what David Bishop sees as the keys to success for the Mid-Atlantic Semiconductor Hub (MASH).

Bishop is a professor of physics, the head of the Division of Materials Science and Engineering, and director of the CELL-MET Engineering Research Center at Boston University. MASH was formed in response to the CHIPS (Creating Helpful Incentives to Produce Semiconductors) and Science Act, which is focused on boosting domestic production of semiconductors and related technologies. It is a regional hub consisting of a partnership among 10 universities including Penn State and Boston University, and various industry and government entities.

Bishop brings a unique perspective to the table, as he has a career that includes 33 years working for Bell Laboratories and 12 years at Boston University.

“I would say as an individual, I really understand the world from both perspectives, having kind of been in both domains,” Bishop said. "One of the key things about the CHIPS Act is trying to enhance the competitiveness of the American semiconductor industry. To do this, academia needs to forge an effective partnership with this industry.”

Part of this is communication and understanding each other's perspective, goals, and needs. This, Bishop said, can be a little difficult due to each group not knowing the other's world very well, such as the culture and how things are done differently in academia and as opposed to industry.

> "There's real value in having some members of our team who understands both sides and can build bridges between the two sides,” Bishop said. “We then realize that even though the goals may be the same, there are different cultures, different ways of approaching it, different ways of thinking about how to solve problems. It leads to an understanding that this is a win-win scenario, and we can leverage each other's strengths.”

The MASH universities themselves boast a wide range of strengths, including robust material research and other

Credit: Adobe Stock

STEM programs and state-of-the-art facilities. Their focus on areas such as infrared detectors, nano manufacturing, low-energy computing, and power computing are key to semiconductor work. However, Bishop said that the MASH universities can add another important aspect to this effort: workforce development.

Building America's semiconductor industry back to its prior prominence will require tens of thousands of skilled workers. This is a major focus of the CHIPS Act. Bishop notes that to find qualified workers, semiconductor companies and universities need to partner on early education programs such as Boston University's Engineering Engagement Kit (EEK), which introduces elementary school students to the concept of engineering and inspires them to pursue STEM careers.

"If you ask a five-year-old what an engineer is, a five-year-old thinks the engineer is the person who drives the train and does not know that the engineer is the person who built the train," Bishop said. "The EEK introduces the concept of what engineering is and what engineers do to show them that engineering is an interesting, important way to change the world. It plants the idea early of engineering as a career. A lot of students, especially those in underrepresented populations, who could become engineers will not do so if they are not given the right kind of encouragement or opportunities"

Encouraging these underrepresented communities is important for the future of America's semiconductor industry simply because of the number of workers that are needed as it ramps up to levels outlined in the CHIPS Act. Bishop stressed that the net for workers needs to be cast with diversity in mind and include underrepresented communities.

"Every industrial company looks around, looks at their workforce, and realizes that it's not as diverse as it should be," Bishop said. "I think by partnering, we can put together a good workforce that's diverse with broad participation, one that creates innovative technical solutions and valuable intellectual property."

MASH is designed to leverage the unique strengths that individuals and institutions within higher education, industry, and government bring to the semiconductor industry. As Bishop stresses, by combining the expertise of diverse stakeholders, fostering collaboration, and listening to each other, universities can play a pivotal role in strengthening the American semiconductor industry.

"MASH will be a wonderful team to be a member of," Bishop said. "I'm really excited to be part of this team and excited to work with these individuals to show the world what we can all do." ■

Ceramics and Glass: A new vision for ancient materials

Credit: Adobe Stock

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CERAMICS AND GLASS are two materials that have been around since ancient times, yet many people outside of materials science are unaware of the impact they have on their lives beyond the obvious.

They truly have a long history. The oldest known instance of ceramics is believed to be the Venus of Dolní Vestonice, a figurine of a goddess found in what is today the Czech Republic. It dates back to around 28000 B.C. and is an example of ceramics as art. Glass, for its part, is relatively “younger,” with the earliest examples of man-made glass found in Mesopotamia and Egypt around 3500 B.C.

Both materials evolved over the centuries and quickly found familiar roles in our society. Glass was made by melting silica, soda, and lime in a fiery furnace and was originally used for decorative purposes, such as jewelry or mosaics. Eventually, glass was used in windows, and often could be quite beautiful, such as the stained-glass windows used in Middle Ages churches that survive to this day.

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As the Industrial Revolution of the 19th Century ushered in a new era, glass found new uses. Mass production enabled lower cost windows, eyeglasses and mirrors, and advances in optical glass drove development of glass innovations such as new and better lenses for telescopes and microscopes. At the end of the century, growing use of electricity raised demand of the newly invented glass incandescent light bulb.

Glass technologies raced ahead in the 20th Century, as new development of new types of glass such as laminated, tempered, and wired cast glass enabled new ideas in architectural glazing, with "all-glass" skyscrapers becoming a larger and larger part of city skylines. As the electronic age dawned, glass played a significant role with glass fiber optic cables transmitting voice and data across the globe at remarkably high speeds. The creation of strong glasses such as Corning's Gorilla Glass, developed in part by Penn State faculty member John Mauro, has put glass in our pocket in the form of smartphones.

Ceramics, on the other hand, have also evolved from everyday uses such as food and water storage in ancient times to a growing "behind the scenes" role in our everyday modern lives. As ancient civilizations in places such as Greece and China became more sophisticated in their ceramic production, ceramics became both practical and artistic. For example, intricate Chinese porcelain vessels from centuries ago survive to this day in museums as a testament to both the practical and the beautiful.

Like glass, the Industrial Revolution was a real game-changer for ceramics. Factories took advantage of new techniques and technologies like steam-powered engines to mass produce ceramics ranging from china and other housewares to building materials such as cement and concrete (which are in fact ceramics).

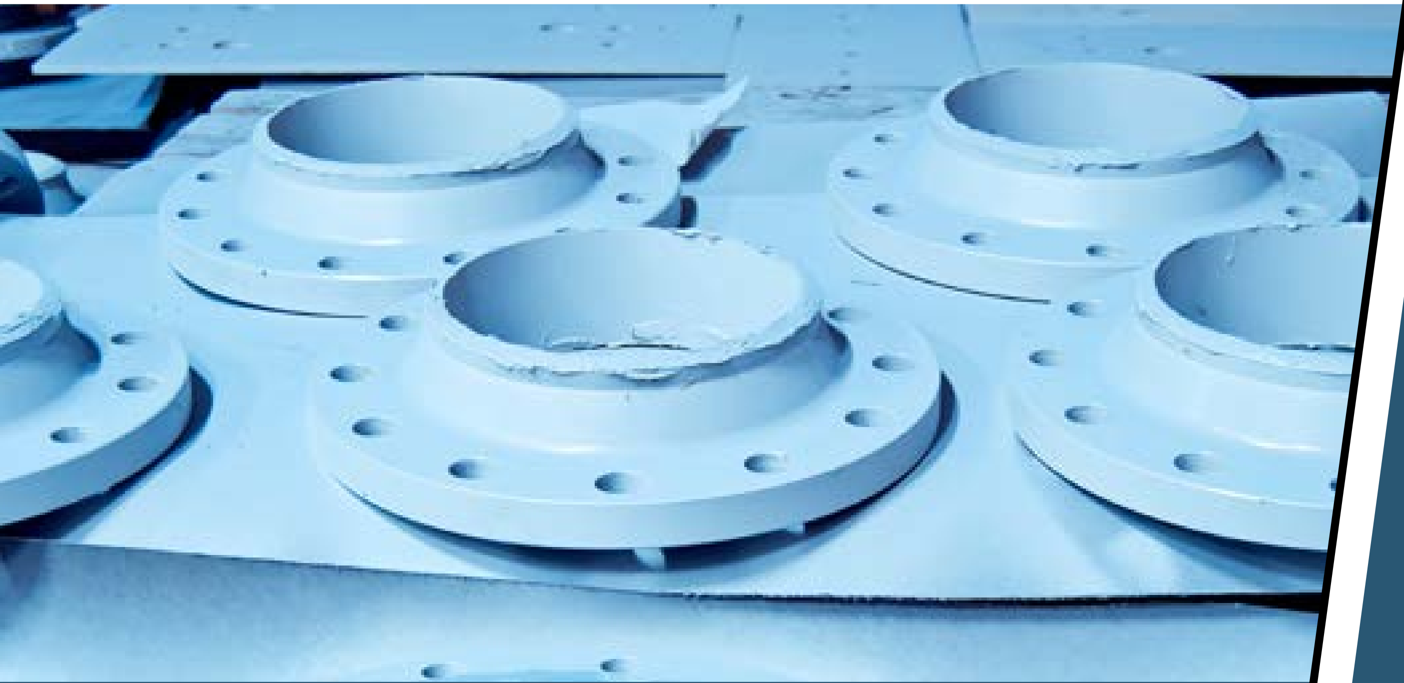
Today, ceramic technology is advancing fast, including research carried out at the Materials Research Institute (MRI) and other areas around Penn State. Ceramics can be 3D printed, enabling new ceramic designs. Ceramics hold potential as materials for energy storage, and even energy creation through processes such as piezoelectrics and ferroelectrics. Ceramics work well within the human body, giving ceramics a huge role in biomaterials such as bone implants and artificial joints.

Some of these advances were carried out at Penn State. For example, retired director of MRI, Carlo Pantano, is considered a pioneer of modern glass research. His ground-breaking work ranged from using glass for safe long-term immobilization of nuclear waste to lab-on-a-chip technology to renewable energy. For this legacy, he was awarded the George W. Morey Award for new and original work in the field of glass science and technology in 2005.

On the ceramics side, Della M. Roy carried out research at Penn State that was so impactful, it enabled her to become the first woman elected to the World Academy of Ceramics. Her work around the engineering of cement and concrete included developing porous biomaterials for bone repair and chemically bonded ceramics, just to name a few.

In this issue of Focus on Materials, we look at innovative glass and ceramics research being done at Penn State. This includes research on building housing for future inhabitants of the Moon and Mars, methods of manufacturing glass and ceramics at a much lower carbon footprint, the role of these materials in brand-new field of regenerative medicine, and more.

While both materials have been around for thousands of years, humanity has not finished exploring their potential. And that is especially true at Penn State. ■



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How ceramics changed the piezoelectric game

CERAMICS HAVE A lot of uses in our society, from artistic vases to construction materials to solid-state batteries, but one of the most interesting applications of ceramics is as piezoelectric materials.

Piezoelectric materials generate an electric charge when rapidly compressed by a mechanical force during vibrations or motion, which makes them useful as sensors. They also deform and change in shape when an electric field is applied, which makes them useful as actuators and transducers. They can also be used to scavenge power from motion, for applications ranging from self-powering sensors to personal electronics such as wristband devices.

The discovery of ceramics as a piezoelectric material was something of a happy accident.

"R.B. Gray, who was working at Erie Resistor Corporation in the 1940s, was the first person to recognize that a ceramic material could be poled and made piezoelectric," Susan Trolier-McKinstry said, Evan Pugh University Professor and Flaschen Professor of Ceramic Science and Engineering. "And the story the late Professor L. Eric Cross used to tell is that he left a barium titanate ceramic under a DC electric field overnight, and when he came back in the next morning it was humming. And it was humming because he was applying a small alternating electric field to it, and it was oscillating in a frequency that the ear could hear.

"And that's how they first discovered that you could make piezoelectric ceramic materials and generate a net piezo electric effect by poling them."

This discovery was significant because of the microstructure of piezoelectrics. Ceramics are polycrystalline, and can often be prepared at much lower cost, than single crystal piezoelectric materials.

"Until ceramics were found to be piezoelectric, it required a single crystal, which means that I have to grow a special orientation crystal and it tends to be time intensive," Trolier-McKinstry said. "So, the ability to short circuit that process and make a ceramic which can be stamped out on a pellet press was revolutionary in terms of reducing cost and the enabling a wider range of applications."

"Polycrystalline materials can be made much less expensive than single-crystalline materials," Trolier-McKinstry added. "The cost differential is enormous because a comparable volume of a ceramic might cost a penny compared to a lead magnesium niobate – lead titanate single crystal, which can cost between $10 and $100 for a similar size. Ceramics are easier to make shapes with, including unusual shapes."

Trolier-McKinstry's research focuses on piezoelectric thin films. The advantage of piezoelectric thin films is they can be driven at a much lower voltage than other piezoelectric materials.

"So, I get the same electric field but at a few volts, which just simplifies the electronics system," Trolier-McKinstry said.

These small-size, thin piezoelectric materials open the door for many potential applications. For example, Trolier-McKinstry is working on making miniature medical ultrasound systems the size of a thumbnail, which would be ideal for body cavity-based imaging. Additionally, she is working on making miniature sensor systems for balance for athletes and the elderly. The sensors would be embedded in shoe soles and would be important for athletes who need to improve their running technique to minimize future injuries.

"For the elderly population, one of the major medical risks is falls," Trolier-McKinstry said. "So, if you can sense someone's balance, literally know when they are becoming wobbly, that could be very useful. Right now, it is measured in doctor's offices very infrequently and typically right after a medication regime when people are most likely to be most steady. So, we have a lot of interest in making something easy to wear that could alert people that their balance is not good, and they need to sit down or take medication to improve their balance."

Adjustable optics is another area of research in piezoelectric ceramics. Trolier-McKinstry is working on making adjustable optics that are being considered for the proposed Lynx X-Ray space telescope. The adjustable optics could also be used to provide high-resolution images of materials and biological specimens.

"This telescope's optics requires very precise shapes, which will either have to be made in a material that's polished to shape and is extraordinarily stiff, so you can't bend it," Trolier-McKinstry said. "Or we need to be able to fix the deformations that happen. And so, we are working on fixing those deformations. We really do lots of work developing different types of devices that utilize that piezoelectric effect."

As for the future of piezoceramic materials, Trolier-McKinstry sees a couple of areas that are poised for big changes. The first is in bulk piezoelectric ceramics, which historically have had many grains, all of which have had random orientations. There is now worldwide interest in replacing those with materials that are textured, so they are intermediate between a random polycrystal and a single crystal.

> "Single crystals are very expensive, but their properties are very nice, and the random ceramics, they're very inexpensive, but the property trade-off exists," Trolier-McKinstry said. "But if we can sit in a sweet spot in the middle, where there's potential for real applications, that would be one area where I think we're kind of poised for significant growth."

A second area is in the general field of piezoelectric microelectromechanical systems, which employ piezoelectric thin films. This also uses the same type of processing techniques widely used for semiconductors.

"This allows you to do mass batch fabrication and at much finer scales than has been done previously," Trolier-McKinstry said. "There's certainly lots of companies looking at this for virtual reality and augmented reality goggles. Likewise, there are many companies that are working on being able to take medical devices and make them ubiquitous for anything from pulse monitors to wearable ultrasound systems. We are at the point where the field is starting to explode in terms of commercial production."

All these new innovations mean that piezoelectric ceramics are primed for a bright future. ■

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Creating a new kind of super-hard ceramic through machine learning

RESEARCH ON CERAMICS at Penn State has become rather spicy lately. Spinodal-hardened high-entropy ceramics, also known as SPICES, extend high-entropy ceramic development into a new category.

Research into these ceramics is part of a multi-university project that includes Duke University, the University of Buffalo, North Carolina State University, Missouri University of Science and Technology, and Penn State. Each university brings its own unique expertise, ranging from computational predictions and machine learning algorithms to bulk high entropy ceramic development and thin film exploration.

High-entropy ceramics are a special class of ceramics composed of at least five components in significant proportions. This blending of different materials under suitable conditions leads to formation of alloys with high configurational entropy, which is entropy or order of a system that is due to the location of the constituent particles.

“This means the level of atomic randomness or disorder is substantially higher in these materials compared to more traditional ceramics, as the potential number of configurations to arrange these five components together is substantially greater than simpler systems, such binary alloys,” said Douglas Wolfe, professor of materials science and engineering, professor of engineering science and mechanics, professor of nuclear engineering, professor of additive manufacturing and design, and the head of the Metals, Ceramics and Coatings Processing Department of the Applied Research Laboratory (ARL). “In other words, high-entropy ceramics are unique, complex mixtures of ceramics that dissolve into each other to form new materials which have never been developed before.”

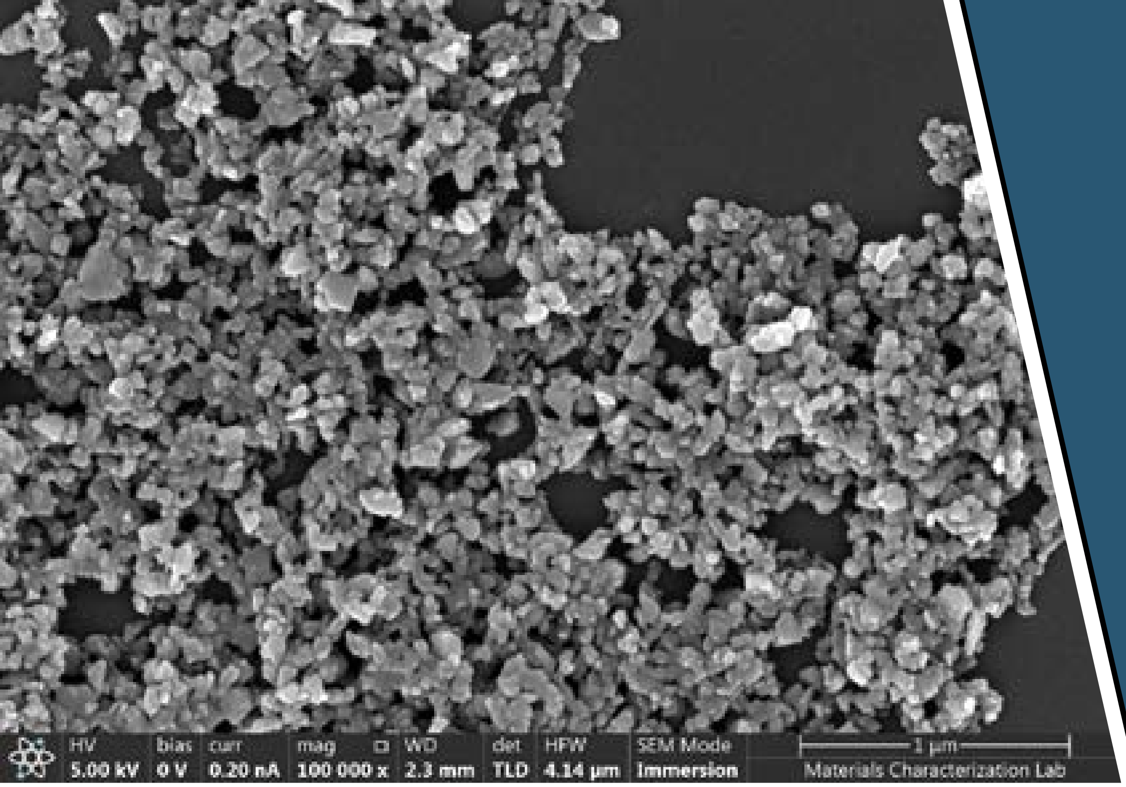
Spinodals refer to a type of phase transformation that creates a composite structure that can be described as spaghetti-like.

“The entangled composite structure combines multiple hardening or strengthening mechanisms together, such as solid solution strengthening and interfacial coherency effects between the spaghetti-like regions,” said Jon-Paul Maria, professor of materials science and engineering. “This spinodal-hardening provides an effective means to strengthen materials beyond their conventional limits.”

Along with their unique composition, SPICES also involve machine learning in their design. Machine learning helps researchers overcome a major challenge in developing these high-entropy ceramics. With at least five different components across multiple types of ceramics, there are an infinite number of compositions possible.

> “Of these infinite compositions, there is a much smaller subspace of spinodal-viable compositions,” Wolfe said. “To experimentally test every potential composition would be too infeasible, especially considering the limited experimental insights into spinodals beyond two components, let alone five.”

This is where machine learning becomes near-essential to their work. The use of machine learning in guiding compositional design, screening, and material predictions is an extremely valuable tool to efficiently navigate this unique high-entropy landscape.



Spinodal-hardened high-entropy ceramics have applications ranging from manufacturing to defense
Credit: Doug Wolfe

"Furthermore, this machine-guided approach allows for further prediction and filtering of candidate materials based on calculated mechanical properties such as stiffness, hardness, and deformation mechanisms, and thermal properties such as melting point, thermal expansion, and phase stability to provide the best candidates to evaluate for superhard or ultra-high temperature applications," Maria said.

The societal benefits and applications of SPICES are potentially wide-ranging and many.

"The improved thermomechanical properties and performance of these ceramics have the potential to exceed conventional, state-of-the-art materials," Wolfe said. "These materials can be used for wear-resistant applications, such as sharp cutting tools, friction-stir welding, and rotating/sliding assemblies. Additionally, their improved high-temperature properties make them highly suitable for aerospace and hypersonic applications, where durability to erosive debris and stability under extreme conditions is critical."

So far, SPICES researchers have established several baseline experimental studies and have successfully developed multiple material systems to validate their latest computational models. The next steps include expanding their spinodal-viable candidate materials list efficiently with new experiments and advanced screening methods to further explore this uncharted research territory.

"From there, refined characterization and ranking of these spinodal-hardening effects on enhanced thermomechanical properties will be applied accordingly to ultimately evaluate the best SPICES materials for Department of Defense applications of interest," Maria said.

The SPICES research effort is paving the way forward in investigating new entropy-driven materials design and spinodal-hardening. This research supports multiple key technological areas, ranging from traditional industrial/manufacturing components to extreme leading-edge hypersonic developments. The collaboration between these universities has the potential to revolutionize materials science and pave the way forward for new, advanced ceramic materials. ■

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The bright future of ceramics as a biomaterial

CERAMICS HAVE AN exceptionally long history as a biomaterial. In fact, going back to the existence of vertebrates.

Yes, vertebrates. While this may be surprising to some people, bones are at least partially ceramic.

"Bone is a nano composite ceramic," said Dan Hayes, biomedical engineering department head and Dorothy Foehr Huck and J. Lloyd Huck Chair in Nanotherapeutics and Regenerative Medicine at Penn State, said. "Collagen is the polymer portion of it. But there is a native ceramic that occurs in there called hydroxyapatite. That is the primary form. There are other forms, but it makes up the largest mineral fraction of your bone, and it is an incredibly important component to providing strength and durability of our bones."

Given these facts, it should not be surprising that the first instance of human-engineered bioceramics was related to bones. These early bioceramics were engineered to mimic the native structure and composition of bone to promote bone formation and regeneration.

"This involved either making powders or three-dimensional structures that were used to replace bone and promote bone regeneration, and they've been incredibly successful," Hayes said.

Hayes' focus of ceramic research is on regenerative medicine, including work related to bone medicine, and ceramics are poised to play a significant role.

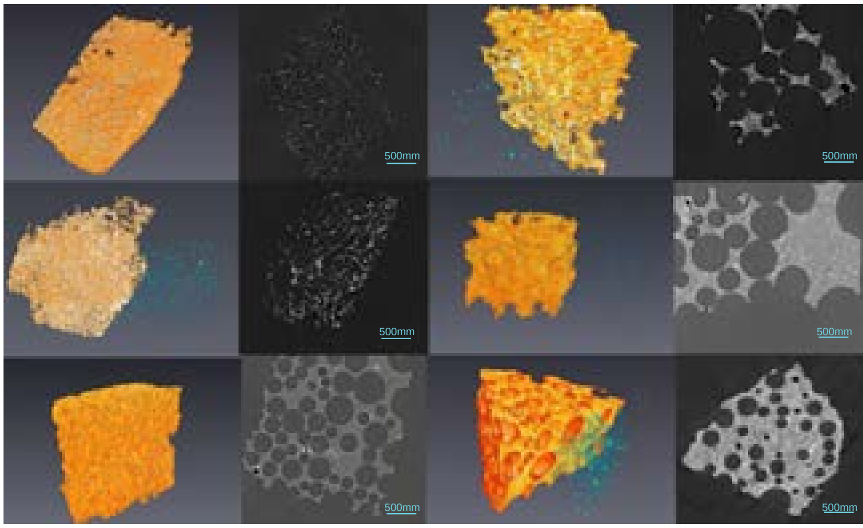
"In tissue engineering and regenerative medicine, we are using these ceramic composite materials to accelerate bone regeneration and other musculoskeletal tissues," Hayes said.

"One of our grand challenges in musculoskeletal tissue regeneration is repairing tissue interfaces, the areas where two tissues come together. Think for example about the articular cartilage in your knee."

Hayes notes that a lot of people have articular cartilage problems, and treating this is difficult because scientists have found it challenging to regenerate articular cartilage. One of the major reasons is that the repaired cartilage is unstable. This is because once it is torn off, it is almost impossible to get it to adhere to the bone again.

> "The issue is that it didn't develop as two different materials, it developed as one material and it's a gradient material," Hayes said. "And it goes from a high ceramic content composite (bone) to a high polymer content composites (cartilage) as a relatively smooth grade. It is not two things that are stuck together, it develops as one material, and as a graded material. The advantage to using micro and nanoscale ceramics is that it allows you to recapitulate that native structure. We can grade it from high ceramic content to low ceramic content, recreating the gradient of mature tissues."

Along with bioactive ceramics, there are also bioinert ceramics. Ceramics that do not have a lot of biological function can more easily be inserted into the body. Their properties, such as refractiveness, stability, and hardness, make them useful for applications such as hip implants.



Uses for ceramics as a biomaterial include improving the success of bone grafts and as a superior material for hip implants. Credit: Dan Hayes

At the same time, ceramics can be made to be bioactive, by adding strontium, magnesium, or silicon. That gives us a vast range of opportunities for ceramic use in the body.

“I am on the regenerative medicine side of this research area, and I am specifically looking at the development of bioactive bioceramics and composites for regenerative medicine,” Hayes said. "The reason I was talking about the osteochondral interface, that articular cartilage interface, because that's where our area of research is. Basically, how do you use bioceramics as part of a material that promotes the development of this native gradient and regenerates it.”

These bioceramic materials and their applications hold immense potential to improve quality of life, especially for elderly populations. They improve the success of bone grafts and bone substitute materials, enabling better solutions for patients.

One example is improved design of hip implants. Longevity is a primary concern when it comes to hip replacements. With an aging population and younger individuals requiring hip replacements, the demand for implants with extended lifespans is increasing. Ceramics, with their durability and longevity, offer an ideal solution for hip implants, reducing the need for revision surgeries and enhancing patient outcomes.

"You want to get one hip implant in your life, right?" Hayes said. “Because you do not want it to wear out and have to get another one. Let us say you get one when you are 70. And it wears out when you are 80 something. Doing a major surgery on an octogenarian is not trivial.”

Hayes added that hip implants are also being inserted into younger patients, and that adds to the importance of ceramics as a long-lasting biomaterial.

“I gave the example of a 70-something person but we're also giving hip implants to 50-year-olds,” Hayes said. “So, we need to have a design lifetime that is not just 10 years. It has to be 25 to 30 years. And ceramics are a wonderful material for longevity.”

As far as what is on the horizon for bioceramics is concerned, Hayes said that additive manufacturing, or 3D printing, is a potential innovation point. Printing bioactive ceramics would greatly enhance the customization of medical implants and devices. Researchers at Penn State are on the forefront of this developing technology, using already existing expertise and research facilities at the University around additive manufacturing technology and ceramics knowledge.

“A bit of a shameless plug about Penn State here, but our ceramics knowledge and our additive manufacturing technology is something we can really leverage for research,” Hayes said. “We have to figure out how we can make additive manufacturing of bioactive bioceramics work, but the ability to use 3D printing to make personalized medical devices for patients would be quite a gamechanger.” ■

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New center focuses on semiconductor packaging, and glass plays a role

Credit: Jennifer M. McCann/Penn State

PACKAGING IS ONE of the final steps in manufacturing an electronic system consisting of semiconductor chips. While it provides protection to prevent degradation of the chips, its main role is providing an interface that can combine and connect other chips to each other.

This is gaining in importance due to increased demand for more power and lower processing costs. New developments like artificial intelligence and the Internet of Things (IoT) make this demand for better packaging even more urgent.

One of Penn State's newest research hubs, the Center for Heterogeneous Integration of Microelectronics Systems (CHIMES), is working on ways to address this growing need by improving communication bandwidth density between chips while lowering energy consumption. The center is a joint effort among 14 universities and led by Penn State. Madhavan Swaminathan, head of Penn State's Department of Electrical Engineering and William E. Leonhard Endowed Chair in Penn State College of Engineering's School of Electrical Engineering and Computer Science, will direct the center.

Swaminathan explained that the center is exploring ways to collect data from edge devices and process it efficiently.

"What we are trying to do with the center is to find ways by which we can increase the bandwidth density in terms of communication between chips and do it at a very, very low energy consumption," Swaminathan said. "And then we can look at applications related to edge computing and distributed computing."

Swaminathan stresses that the key to efficient processing lies in packaging, and that interconnecting chips from different technologies and processes can achieve this. One of the goals of CHIMES is to develop ways to interconnect chips from various processes and technologies to create smaller chips that can be connected to each other. This method, called heterogeneous integration, will reduce the cost of integration within a single chip, leading to more efficient computing.

"It turns out that packaging plays a very, very important role, and that is where heterogeneous integration comes in," Swaminathan said. "Heterogenous integration is where you're interconnecting chips from various processes and from various technologies together in a way where you can place these chips very close to each other. So, doing all your integration within a chip can be very expensive. The idea here is how do you break it up into smaller chips that can then be connected to each other?"

To drive home the importance of packaging, Swaminathan gave two real-world examples of applications. One is in communications, using modern automobiles as a case in point. An automobile has become an IoT device on wheels, moving all over, collecting data and transmitting that data to communicate with other devices, such as Google Maps or other elements of the vehicle such as sensors and steering components. A potential bottleneck to this process how much data these devices are able to transmit and receive.

> "In our mobile networks we've gone from 2g to 3g to 4g, and today it's at 5g," Swaminathan said. "While 5g gives you a certain amount of data speed, let us say we want to multiply that data speed by a factor of 10. Packaging plays a particularly important role in terms of able the ability to be able to support communication devices like this."

Another example is dealing with the amount of heat that is generated when a processor is running at a high speed. The problem would become worse as processors become faster.

"Imagine trying to increase the speed of the processor by two orders of magnitude, just imagine the amount of heat it is going to generate," Swaminathan said. "That is not sustainable, right? Because you need to find a way to dissipate that heat or figure out other ways by which you can package these electronics so that it dissipates that level of heat. So, that is where packaging plays a role in trying to distribute this heat in a way so it can be easily removed."

Swaminathan said that CHIMES will explore glass as a potential packaging material.

"If you look at the way advanced packaging is being done today, it is by making use of silicon," Swaminathan said. "Silicon has some challenges, but more importantly, these silicon-based solutions are being practiced by companies outside of the United States."

Swaminathan noted that the organizational goals of CHIMES run parallel with some of the goals in the CHIPS and Science Act, which was a $52 billion investment in semiconductors signed in 2022 by President Joe Biden. The investment focuses on increasing onshoring of manufacturing and U.S. leadership in the microelectronics industry. Currently, most semiconductor development and manufacturing occur overseas, especially in Taiwan. Glass packaging material could be a key development for bringing more semiconductor manufacturing into the U.S.

"We want to onshore a lot of the packaging solutions and include that in American manufacturing," Swaminathan said. "When you think about restoring U.S. leadership in chips, what should we focus on? One of the potential solutions is glass packaging. The idea here is to build your packages by replacing silicon with glass, then add polymers on either side of it, along with metallization. Then embed chips into this packaging. You can build a very compelling case for this kind of packaging, especially when it comes to high-speed wireless communication. Glass can play a very, very important role."

Penn State, because of its relationship with major players in the glass industry, is well-positioned to drive such glass-related innovation.

"The reason this is so important for Penn State is because of our relationship with the likes of Corning and Schott Glass," Swaminathan said. "Schott Glass has a facility in Pennsylvania, and Corning is a company that Penn State has been working with very closely. These are opportunities for us in terms of being able to build an ecosystem where a lot of the glass packaging research that we do within CHIMES can find its way into manufacturing."

The CHIPS Act has a five-year timeline. But CHIMES' research aims to develop new ideas that can be transitioned into manufacturing and will play a crucial role in achieving sustainability beyond the five-year CHIPS Act timeline. CHIMES is looking at a ten-year horizon, not just a five-year timeline, and hopes to bridge the gap between its research and the near-term needs of the CHIPS Act. By partnering with other universities in the development of new technologies, Penn State and CHIMES can be a leader in semiconductor packaging and workforce development. ■

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Architectural glazing for energy savings, and better health

Credit: Adobe Stock

ARCHITECTURAL GLAZING IS more than just a way to create a beautiful building. In a world affected by climate change and focused on saving energy, windows are extremely important beyond just offering building inhabitants an easy way to quickly check the weather outside.

Given windows are a weak link for energy concerns since they are the most exposed part of a building, it is crucial to focus on energy-efficient window designs. However, architectural glazing is not only about fenestration, which is the design of placement and number of windows on a building, but it is also related to the entire building facade. And it is also very important for the comfort and well-being, both mentally and physically, of the people occupying the building.

The research of Julian Wang, associate professor of architectural engineering, is focused on making architectural glazing more dynamic, energy-efficient, and human-friendly.

"The most straightforward impact of architectural glazing is about energy savings," Wang said. "But we have to keep in mind the occupants of buildings, so we need to consider how windows affect their behavior, comfort, well-being, and even health."

Wang and his research group, the ArchiLambda Lab, has three primary perspectives on the glazing system: the glazing itself, human factors, and the environmental factors. His lab works with fellow materials scientists at Penn State and at other institutions on finding ways to make architectural glazing systems more energy efficient.

> "Currently, buildings are responsible for around 40% of primary energy consumption, and 36% of total carbon dioxide emissions," Anwar Jahid, post-doctoral researcher in Wang's lab, said. "It was our primary goal to develop smart windows that would enable less energy consumption inside the building."

The key to this, according to Wang, was thinking a bit outside the box.

"There are a bunch of different ways to make glazing systems more energy efficient, for instance, we could add like a silica aerogel or some other highly insulating materials into the glazing," Wang said. "But we're doing a little bit different way, we're trying to make our architectural glazing system one that can actively and dynamically respond to external weather conditions."

External weather conditions in this time of climate change can be extreme. To address these extremes, they are working on developing energy-efficient glazing systems that can respond dynamically to external weather conditions by incorporating nanoscale materials. This involves adding films and nanoscale materials that interact with light to control solar penetration through windows, depending on factors such as the season, solar position, sky conditions, and location.

“We intuitively understand in summer we don't want a lot of sun penetrating and in winter, we do want sun penetrating the window,” Wang said. “You could close the blinds or have some other shading system, but we developed a thin, barely visible nanofilm made with light-interactive material that can selectively respond to solar rays, including times when the solar position is higher or lower depending on time of day or season and cloudy days.”

The researchers found that their results were promising as far as energy savings.

"We demonstrated the potential for energy savings to reach over 18% in a mixed climate, areas that have a cold winter and a hot summer, compared with using the most recent energy efficient standards,” Jahid said.

While energy savings is important, Wang again empathized the need to weigh effects on the building’s occupants. So, the team’s research considers both science and human factors. He notes that you can feel the importance of architectural glazing just by standing in front of a window on a hot summer day when the sun is blasting heat into the structure.

"Such conditions can change human behaviors, affect worker productivity and so on, and this is because architectural glazing can greatly affect human visual and thermal comfort,” Wang said. “So, our work is also about indoor environmental quality, and human well-being, as well as being about energy savings.”

Wang is also working on another architectural glazing project that involves human well-being: how light affects dementia patients in nursing homes. Wang is partnering with Ying Ling Jao, associate professor of nursing at Penn State to investigate whether combining architectural glazing with indoor electrical lighting systems can improve dementia symptoms. They focus on the impact of different lighting conditions on the behavior of people with dementia and are finding that lighting through glazing systems could play a critical role in mitigating these symptoms.

“We are working to understand whether we can characterize some glazing systems for architectural applications within nursing homes,” Wang said. “This endeavor would combine that with the inside lighting system and be implemented to enhance the living conditions for older residents, particularly those suffering from dementia. We are aware that exposure to different lighting conditions affects their behavioral symptoms. Consequently, we theorize that the specification of glazing systems in a senior care facility may also play a pivotal role in their health.”

Wang noted that there were challenges to overcome in bringing this theory to reality.

“However, we recognize the inherent complexities associated with the varying daily and seasonal changes in outdoor solar light and sky conditions, as well as differences between building facades,” Wang said. “The daylight transmitted through window systems does not always align with the interior lighting needs required to support optimal circadian health. In response to this challenge, our research is concentrated on developing strategies that adapt to these natural light variations, with the goal of better catering to the circadian health requirements of the elderly within nursing homes, particularly those suffering from dementia.”

It is a new frontier for Wang’s research, one that looks at architectural glazing for something more than just an attractive-looking building and a nice office window to look out of.

"We think about architectural glazing for energy solutions, and also, we also think about it from the human perspective,” Wang said. “We want to help with human comfort, and human health.” ■

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Ceramic batteries to power a new world

WHILE CERAMICS HAVE been used as a battery material for decades, ceramic battery materials are having a moment right now.

With climate change concerns only growing, the use of ceramics as an advanced electrode or electrolyte garners interest because of the possibility it could enable more compact, safer, and longer-life batteries for applications in electric vehicles and grid energy storage.

“For example, ceramic coatings for cathodes can improve the stability and durability of electrodes, reducing degradation and increasing overall performance,” said Donghai Wang, professor of mechanical engineering.

Ceramics also hold a lot of promise as a material for solid state batteries. 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 several advantages over liquid electrolyte batteries.

“Ceramic materials can be used as solid-state electrolytes to replace conventional liquid electrolytes, which are flammable and can leak or explode,” Li-Ji Jhang, doctoral candidate. “Also, solid electrolytes have higher thermal stability, which means they can withstand high temperatures without degrading or losing their properties. In addition, they can be in a relatively small volume when packaged properly, which can largely increase the energy density of the battery.”

There is also another positive aspect to these types of batteries: They are sustainable.

> “Many ceramic materials are environmentally friendly, which makes them an attractive option for sustainability,” Wang said. “Overall, the development of ceramics as a battery material is an exciting area of research with the potential to transform battery technology. In short, the solid-state electrolyte can offer improved safety, higher energy density, and longer cycle life for battery applications.”

Wang’s lab has been at the forefront of ceramic battery development, with a variety of research projects.

“We are working on the development of glass-ceramics solid-state electrolytes for all-solid-state Na-S batteries,” Jhang said. “The ionic conductivity of solid electrolytes is another

Credit: Adobe Stock

important feature we need to consider. Most solid electrolytes in sodium solid-state batteries have relatively lower ionic conductivity than 1 mS cm-1, which is also lower than liquid electrolytes.

"In order to facilitate practical all-solid-state batteries, we need to improve their ionic transports within the solid electrolyte. We plan to substitute some cations or anions in Na_3SbS_4 glass-ceramics solid-state electrolyte to increase further its ionic conductivity and chemical stability against the Na metal anode."

Such research is important as a key aspect of the fight against climate change as the world moves away from fossil fuels and toward more electricity as an energy source. Ceramic battery materials could enhance batteries for energy storage in various applications from electric vehicles to consumer electronics, and even to grid-scale electrical storage.

"As the world moves towards net-zero carbon emission, the need for energy storage solutions for renewable energy becomes increasingly important," Wang said. "The ceramic batteries can achieve higher energy density, longer cycle life, and improved safety compared to traditional batteries, potentially becoming a great option for clean energy applications."

Both Jhang and Wang see a bright future for ceramics in battery applications. An important part of the equation is commercialization of this technology. Currently, many ceramic battery materials are still not at the point of scalability.

"Some trends I see in the research revolve around the safety, scalability, and commercialization of ceramic batteries," Jhang said. "One of the major advantages of ceramic batteries is that they are less prone to thermal runaway or explosion. However, many ceramic materials are still on a laboratory scale and are expensive. They have not yet been scaled up for commercial production either. Therefore, to practically utilize ceramic materials in batteries, more research needs to be conducted, and the technology can become more mature and transform the energy storage industry." ■

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Helping glass reach its steely potential

SEEING SURFACE DEFECTS ON GLASS IS KEY

THEORETICALLY, GLASS SHOULD be one of the world's strongest materials. However, as anyone who dropped a drinking glass on a hard surface knows, it breaks easily. It is brittle.

"Glass, in theory, is estimated to be similar to hard steel," said Seong Kim, distinguished professor of chemical engineering and associate head of the Department of Chemical Engineering at Penn State. "But we all know in real life that is not the case. The main reason is because of surface defects. When stress is applied, that stress is focused and localized to the surface defect. Once the surface starts to crack, glass has no grain boundaries, and it propagates all the way through the material so the glass breaks."

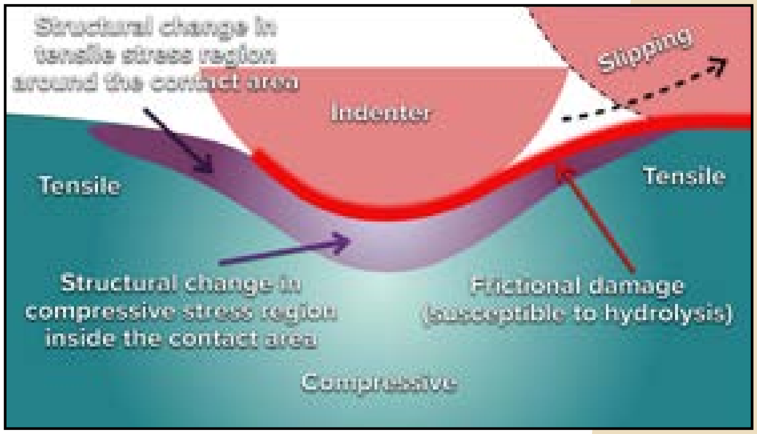
Glass is seemingly not that complicated of a material. Approximately 70 percent of all glass is silicon oxide. Glass is also a material that has been made for thousands of years and is so common most of us do not even think about its presence. Yet, there is still much about glass that is unknown.

"The Roman philosopher Pliny the Elder lived two thousand years ago, and he mentions glassmaking in his writings, for example," said Andrew Ogrinc, doctoral candidate in chemical engineering. "But humans did not have confirmation of what the atoms in a silicate glass looked like until 2012 when researchers used TEM (Transmission Electron Microscopy) to take an image of the silicon atoms in glass. Until then, there was a lot of disagreement about what it would actually look like, which is amazing given how common glass is in our everyday lives."

So, given its ubiquity, creating glass that lives up to its theoretical strength would have many applications. But if surface defects are the main reason glass is not as strong as it could be, is defect-free glass even possible? The first step in answering that question, according to Ogrinc and Kim, is being able to better "see" the defects, and better understand what is going on at the surface of glass. To achieve this, Kim's lab must be innovative because characterizing glass offers unique challenges that other materials do not.

> "The typical surface characterization methods that are widely used for metals and semiconductors do not work for glass," Kim said. "Glass is an insulator so characterization methods that rely on electrons and ions are very difficult to use with glass. And when optical spectroscopy methods are used, the glass is transparent, so the light of course goes through the material. It makes it extremely complicated."

So, the researchers had to get creative.



Schematic illustration of stresses generated during the Hertzian indentation and subsurface structural changes revealed by surface-sensitive vibrational spectroscopy and chemical etching. Credit: Seong Kim Lab/Penn State

“We use spectroscopy and corrosion and mechanical testing to look at how exactly the structure changes and then figure out what that means when the structure has changed,” Ogrinc said. “And then, how does that directly impact the strength and corrosion resistance of the glass? So basically, it’s looking very closely at the surface of glass with a lot of really high-end equipment and then trying to make sense of all these different results together.”

A good example of how important defects in glass are to its strength can be found in Gorilla Glass, Corning’s innovative new form of glass developed in part by John Mauro, who is currently a Dorothy Pate Enright Professor and associate head for graduate education in the Department of Materials Science and Engineering at Penn State and formerly a Corning employee. Gorilla Glass, Kim notes, tests at an extremely high strength when it is first is manufactured and goes downhill from there with time.

“When they make Gorilla Glass and test it, it is at a very high strength; but during transport, it is exposed to a variety of environmental conditions, it touches other materials, and then it becomes not as strong,” Kim said. “If you look at the surface there is no visual damage, everything looks transparent, but it is weaker, so we try to understand why by examining what is going on at the glass surface.”

Glass is often shipped with paper between the sheets of glass and that thought to enable it to remain strong.

“However, our research group rubbed glass with a piece of paper similar to what was used to ship glass,” Ogrinc said. “And then we used a technique called sum frequency generation (SFG) spectroscopy, or SFG, which is shining light on a material and examining how the energy of the light changes. That tells you what the vibrational modes are in the material. If you just look at the glass with your eyes, it looks pristine, no marks, and no changes. But when we look at it with SFG, we see significant changes.”

Along with structural defects, which may happen to your phone’s Gorilla Glass screen when you are swiping and tapping it, the team also reviews chemical changes to glass. While glass being so resistant to chemical corrosion is why it is used for such applications as storing nuclear waste in glass tubes, it still can be damaged by chemicals if it has defects.

“Glass doesn’t rust, and it doesn’t break down like polymers do because it is so inert,” Ogrinc said. “But when we rub the glass with paper or make very shallow indents to create defects, it can still corrode and dissolve at a higher pH. When we put such glass in a pH 13 solution, we can see preferential corrosion where we rubbed the material, demonstrating that even if it does not look different to the naked eye, we need to rely on high-end microscopy to tell us that it is different.”

Being able to see these defects and their effects on the structure of the glass surface is a vital step in developing ultra-strong glass.

“If we want to engineer ways to make glass stronger, first we must understand what makes it weaker,” Kim said. “If we can do that, then in the future, we can help inform designs to fix those issues.

So, thanks in part to this research, perhaps the dream of an unbreakable smartphone screen for those of us who drop them weekly might not be all that far off. However, there are other potential applications, Kim noted. Examples he gave include bioglass applications used in dental implants and improved fiber optics.

"Even with the best fiber optics, if the signal is transmitted, every kilometer, about 4% to 5% of the intensity drops because of the defect in the glass creating fluctuations in the density that scatters the light,” Kim said. “If we need to send a signal from North America to Asia, that is a long distance, so the communication signal degrades. If we can improve the transmission of the signal light through the glass, we can have better fiber optic communications. That is just one example of why defect-free glass would be very valuable.” ■

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The cold sintering revolution continues

AS COLD SINTERING ENDS ITS FIRST DECADE OF EXISTENCE, SCALABILITY IS THE NEXT CHALLENGE

"IN THIS DAY and age, when we have to be incredibly conscious of the CO_2 budget and the energy budget, rethinking many of our manufacturing processes, including ceramics, becomes absolutely vital."

Clive Randall, director of the Materials Research Institute (MRI) and distinguished professor of materials science and engineering said this in 2017, talking about an innovative new process his team developed to sinter powdered materials such as ceramics, known today as cold sintering. Cold sintering's unique and novel process enables sintering in a way that both enables new hybrid materials such as ceramics and polymers and uses much less energy. Today, Randall and his current research team are continuing to study and refine the process.

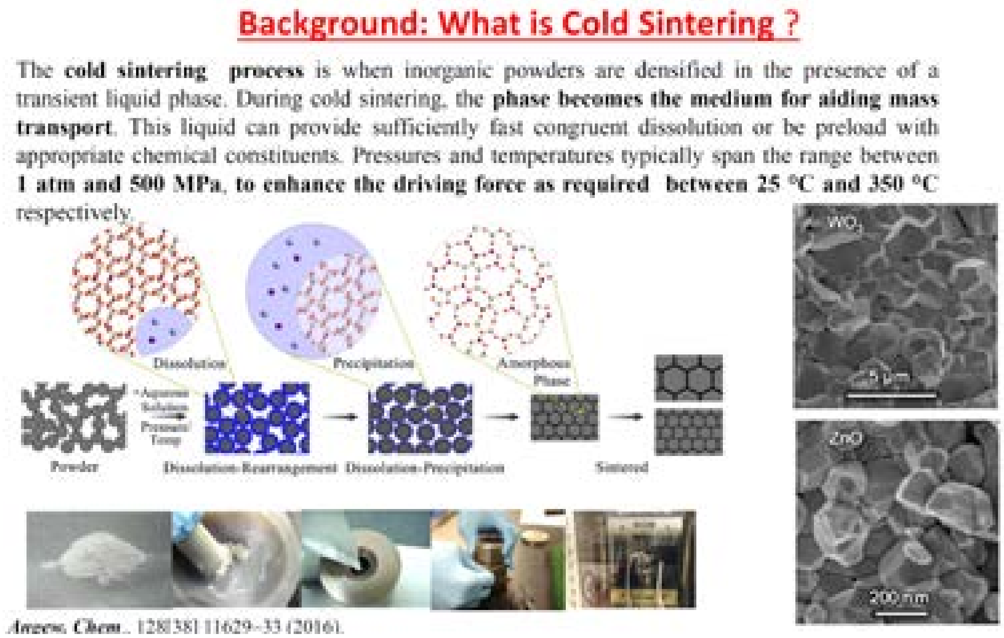
In 2016 and 2017, Randall's group published the first peer-reviewed papers that described a process to sinter ceramics at a range of room temperature up to 300 degrees C. This is much lower than the 1000 degrees C or higher temperatures that are usually required for sintering. The process is also much shorter than traditional sintering which can take hours. Cold sintering requires as little as less than 15 minutes, meaning you can sinter a material in about as much time as it takes to bake a frozen pizza.

In traditional sintering, the powders are heated to very high temperatures until they drive sufficient diffusion, and this permits the powder compacts to form a solid, highly dense body.

The basics of cold sintering involve wetting ceramic powder with a chemical additive that can be water or acid or alkali solutions, which causes chemo-mechanical interactions at the surfaces of the powder particles partially dissolve creating a liquid phase of the ceramic at the particle -particle contacts. Adding temperature and an external critical pressure locally dissolves the contacting solid particles into the liquid at the interface.

There is then a secondary process that happens. The local dissolved clusters of atoms or ions have a concentration gradient and thereby diffuse away from where the particles are in contact. This allows the contacting particles to pack together more tightly and create a solid material. Finally, a third process where there is a re-deposition of the atoms and ions into the pores. The cold sintering process can be rather tricky, as to make it work, a researcher needs to know the exact combinations of chemical additives, pressure, heat, and time necessary for the material to drive all these processes in harmony and reach a high density and strong monolithic ceramic. This can vary depending on the system, as in some systems the process is so simple to carry out that you do not need higher pressures, in others you need to use nanoparticles and/or larger particles.

"There are some general principles around this chemical/mechanical process, and it's all about choosing the right chemistry around that chemical mechanical process for the system that you want," Randall said. "And so, you may have to change things relative to the chemistry of the system, both in the transient phase and in the phases you want to form. There



Credit: Clive Randall

are also a lot of issues regarding the kinetics and how fast each of these reactions occur in different systems. Sometimes you must use a stronger acid or stronger base, sometimes you must use a higher temperature."

Along a process to sinter materials that would have a much lower carbon footprint, the process would enable the creation of composite materials that were not possible before, such as ceramics with organic salts that would hold promise as a battery material. In regular-sintered ceramics, the organic materials would burn off or decompose.

"New processes can revolutionize the making of new materials," Randall said. "Historically, to have a big breakthrough in something you need to have a breakthrough in processing."

This capability, to sinter new ceramics, is important because while ceramics have been around for tens of thousands of years and have been used for food storage and artistic purposes, modern ceramics are highly engineered materials used in anything from high-end batteries, semiconductors, biomaterials such as bone implants, and sophisticated components in engines. The cold sintering process can create sophisticated composite materials for these applications, materials that otherwise would be particularly challenging to impossible to make. For example, through cold sintering, researchers can create ceramic, metal, and plastic composites that can be used in the electronics industry and beyond.

"This is particularly useful for manufacturing printed circuit boards and integrated electronic devices," said Julian Fanghanel, doctoral student in materials science and engineering and part of Randall's research group. "Conventional methods of co-sintering different materials together can be challenging due to thermal expansion mismatch, interdiffusion between components, and unexpected reactions. However, by using cold sintering, we can avoid most of these issues as the temperatures required are too low to trigger these thermal phenomena."

Fanghanel's research in cold sintering is focused on the chemical aspect of cold sintering.

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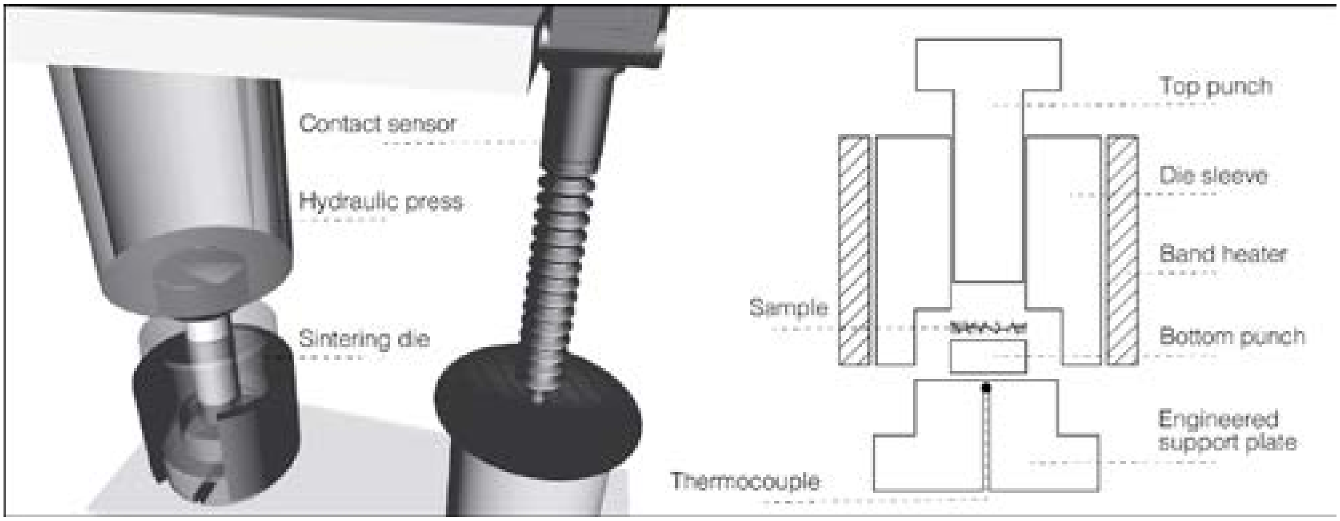

Credit: Clive Randall

“As a chemist, I believe that my perspective can bring a unique approach to the field as we delve deeper into the fundamental mechanisms of cold sintering,” Fanghanel said.

Fanghanel is currently applying cold sintering techniques to developing varistors, thermistors, batteries, capacitors and 5G microwave materials.

“These materials hold the key to faster speeds in our data-driven world, but sintering them using conventional methods is very challenging,” Fanghanel said. “We have made some early progress in developing protocols for sintering these materials using cold sintering, and I believe that there is still a lot of potential in this area of research.”

Fanghanel notes that another significant application of cold sintering is in the production of solid-state batteries, where researchers can join metallic components of the electrodes to an active material such as sodium ion electrolytes. Solid-state batteries hold enormous potential for powering electric vehicles due to being safer and more efficient, however, challenges in manufacturing them remain.

“These materials in solid state batteries can have different thermal expansion coefficients, can react with one another at high temperatures, and even melt at the sintering temperatures of others,” Fanghanel said. “By performing cold sintering at low temperatures, we can avoid these issues while still achieving properties similar to those of conventionally sintered samples.”

Cold sintering is a very new process, and the next step is to scale the process. Right now, Randall notes, they are doing cold sintering at smaller numbers, but his goal is scalability of cold sintering at a level where the benefits of new materials and sintering at a much lower carbon footprint can truly be realized by society. This work is being done in partnership with colleagues at Penn State and from the Montanuniversität Leoben in Austria.

"We're also building on the theoretical understanding of cold sintering and that's an important part,” Randall said. “But I think from a societal perspective, we need to push towards manufacturing. We have done a lot of work in terms of understanding the breadth of the materials that you can cold sinter, and understanding the processes that can come together. But now, probably the most important thing is how you can now take these prototypes into the next stage: manufacturing.” ■

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John Mauro group outside the Steidle building, home to Penn State's Materials Science and Engineering department.
Credit: Mauro group

Gorillas and Lions

JOHN MAURO'S GLASS RESEARCH JOURNEY FROM A CHILDHOOD TRIP TO A GLASS MUSEUM TO CO-INVENTING GORILLA GLASS TO LEADING PENN STATE'S LIONGLASS PROJECT

YOU ARE IN a rush as you run around your house getting ready for work and in your haste, you drop your phone. You hold your breath as you check to see if the screen survived the fall...

...And thankfully, there are no cracks. You breathe a sigh of relief. This sigh of relief is courtesy of Gorilla Glass, the glass that makes up your phone's screen.

Gorilla Glass was developed by Corning Inc., one of leading glass innovators in the world. Gorilla Glass's unique composition is thin, touch-sensitive, and highly durable compared to other glasses. It is used in many electronic devices that include a screen and has saved many a day from being ruined by a shattered cellphone screen.

One of the co-inventors of Gorilla Glass at Corning was John Mauro, who after 18 years at the company brought his prolific expertise to Penn State in 2017. Mauro holds the endowed title of Dorothy Pate Enright Professor of Materials Science and Engineering and is the associate head of graduate education and the chair of the intercollege graduate degree program in the Department of Materials Science and Engineering. He is also leading a project that has potential to be the glass industry's contribution to fighting climate change, LionGlass.

It is the latest chapter in a career of groundbreaking glass research, the seeds of which were planted when Mauro was a child.

"I was six years old, my parents took me to the Corning Museum of Glass, and I fell in love with this material, with its beauty and all the different shapes and colors it could take on," Mauro said. "So that was in the back of my mind. But I did not realize it was a valid career choice until the beginning of my senior year in my high school physics class."

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During that influential physics class, Mauro saw a video produced by nearby Alfred University, titled "What Is Ceramic Engineering?"

"It was from a professor at Alfred named Alexis Clare, who is a glass science professor there, and the video was a Bill Nye the Science Guy type of video that made ceramics and glass a lot of fun," Mauro said. "One of the things that she discussed was glass as a medium for optical computing, like extending fiber optics, but within a computer. After seeing that, everything came together for me with glass. I also loved computers and programming, and I was always captivated by light. It made me realize that this is what I want to study."

Mauro enrolled at Alfred University and combined his love of computers with his love of glass via a double degree in glass science and computer science. During this time, he had two summer internships at Corning, where he worked in the modeling and simulation department writing computer programs that modeled how optical signals propagate along fiber optic communication systems. Mauro received a full-time offer and worked at Corning for two and a half years before going back to graduate school.

"A lot of my first experience with glass research and with research in general was in that industrial environment," Mauro said. "I had a number of outstanding mentors there who taught me the importance of being rigorous in your research."

Mauro returned to graduate school at Alfred and received his doctoral degree in glass science.

"For my Ph.D. research, it was more about modeling approaches for glass structure and for what's called glass transition and relaxation behavior," Mauro said. "What is the process by which a liquid can be cooled into a glassy state? And how does that glassy state relax back to being a liquid if you wait for a long enough time?"

At the same time, Mauro was furthering his research work at Corning, including an effort there to build Corning's capabilities and tools for applying materials modeling towards the design of new glasses. Driven by a desire to get into more hands-on experimental research, he transferred to Corning's glass research department where he had his own lab. This enabled him to do his own glass melting while, at the same time, continue his glass modeling research.

"I could do all my modeling research and then turn that modeling into reality," Mauro said. "I could have the models predict what would be the best compositions and then actually go into the lab and make them. It was a lot of fun taking these glasses from a theoretical prediction in a spreadsheet to a small-scale melt in the lab."

The next steps in this process were going to their factory in Kentucky to do a full-scale trial, sending samples to customers, and finally doing official releases at events like the Consumer Electronics Show in Las Vegas. This was, Mauro said, the approach used for Gorilla Glass.

Mauro soon switched to the management track, overseeing a group of technicians and scientists. He also worked with Penn State graduates such as Rob Schaut, who was the principal inventor of Valor Glass, Corning's pharmaceutical glass product. This was a foreshadowing of sorts of his move to Penn State, which he made in 2017 when he joined the faculty of the College of Earth and Mineral Sciences as professor of materials science and engineering. Today, Mauro is fully immersed as a Penn State researcher and educator.

"At Penn State, my research group has experimental, theoretical, and computational components to the research," Mauro said. "What we want to do is understand how the chemistry of glass impacts its structure, and how that influences its properties. Then we apply that understanding to design new glass and glass-ceramic compositions to enable new applications."

A highlight of this research is LionGlass, which is a new family of glass compositions invented by his research group with a goal of helping to significantly reduce the carbon footprint of the glass industry.

"Although we have developed advanced class compositions like Gorilla Glass, the fact is that at least 95% of worldwide glass production is still standard soda lime silicate glasses: all the architectural windows, the glasses that you drink from, the glass jars at the supermarket, automotive windshields, and so on," Mauro said. "They're all soda lime silicate glass, which is a very old composition that requires melting temperatures of about 1450 degrees Celsius. Hence, it has a significant carbon footprint because of those high temperatures."

In addition, two of the main ingredients used in glass manufacturing are soda ash and limestone, both carbonates. When they melt, the carbonates decompose into oxides, releasing carbon dioxide into the atmosphere. However, LionGlass is different.

"There are two sources of carbon dioxide emissions in glass production: one is the decomposition of carbonates and the other is high energy consumption," Mauro said. "With LionGlass, we eliminate the use of carbonates, so there is no carbon dioxide released from the raw materials."

Also, the LionGlass process reduces the melting temperature by anywhere from 300 to 400 degrees Celsius, depending on the specific composition. The lower melting temperature significantly reduces the energy needed for heating.

"The combined effect is that we can significantly reduce the carbon footprint of the glass industry and make it a lot greener," Mauro said.

Always forward thinking, Mauro peers into the future and sees an increasingly important role for glass in healthcare. He notes that there are already glass compositions for hard tissue repair such as bone replacement and glasses that can help stimulate the body's natural healing process. There are also glass fibers that can help stimulate a diabetic patient's

Dr. John Mauro and Ph.D. student Brittney Hauke running a thermal characterization experiment on their glass Credit: Mauro group

healing process for ulcers, and with the aforementioned Valor Glass, it holds promise for advanced pharmaceutical packaging. There is also an anti-microbial version of Gorilla Glass for touchscreen devices used in hospitals to help prevent the spread of secondary infections.

"Health care is an extremely important opportunity for glass as a bioactive material or a bioinert material that is safe to put into the body, and also as a surface with functionality to provide an anti-microbial environment or safe packaging," Mauro said. "The needs are only going to increase as the population ages, and glass can play a role in ensuring that people can live a long life of the highest quality possible."

Mauro sees these new applications as exciting frontiers for an ancient material.

"Glass is a very old material but it's also one of the least understood materials," Mauro said. "It defies our conventional wisdom with respect to most solid materials - for example, not having a crystal structure. Hence, it poses a lot of unique scientific challenges but also opportunities to apply our scientific understanding towards designing new types of glass in the future." ■

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Combining glass and concrete on the Moon and on Mars

ARCHITECTURE FACULTY MEMBER'S NOVEL WORK IN CONCRETE AND GLASS RESEARCH HOLDS GREAT POTENTIAL FOR SPACE EXPLORATION, AND CLIMATE CHANGE REMEDIATION

THIS ISSUE OF *Focus on Materials* is about concrete and glass. And this article is, in part, about combining the two into one fantastic architectural element.

Shadi Nazarian, associate research professor in architecture, has always been interested in the interdependency among materials, technologies, architecture, and design. This has been a long-time focus of her architecture-related research at Penn State, which includes research to create shelters for explorers on Mars that earned her and her team multiple awards from NASA.

"I have always been interested in glass and in concrete, both considered in the family of ceramics," Nazarian said. "And that these materials could be engineered in response to programmatic and functional requirements. I'm interested in their plasticity, the fact that you can shape them, cast them, and 3D print them to achieve, for instance, functionally graded materials and structures which can exhibit formal continuity with varying performative characteristic."

Nazarian has a glass and ceramics research laboratory at Penn State that explores glass science and technology by experimenting with materials such as molten glass, ceramics, porous glass-ceramics, silica sand, and cement. Her research includes exploring waste materials such as recycled glass, fly ash, and slag. The focus of Nazarian's work is combining concrete and glass in a novel way that enables them to act as an amalgamated material.

"I approached Professor Carlo Pantano, who was at the time the director of MRI, a few weeks after I started teaching at Penn State in spring 2012," Nazarian said. "My unusual research proposal, motivated by an architectural idea, was to develop a seamless and graded transitional interface between glass and an engineered composite material like concrete. With Professor Pantano's support, I met Professor Paolo Colombo of Padova University in Italy, who sent his doctoral student Mauro Marangoni to collaborate with us in achieving this goal in the Transitional Material Interface Laboratory (TMI). I had founded TMI Lab in 2014 with the goal to explore my ideas towards reducing the number of complex joints in buildings."

To unite glass and concrete seamlessly without any mechanical frame to hold glass in place, such as in a concrete wall, Nazarian's lab had to engineer a type of concrete with a coefficient of thermal expansion that would match CTE of glass. This type of concrete, called geopolymer concrete, is friendlier to the environment than traditional concrete because it uses industrial by-products like fly ash and slag to create a binder, resulting in a lower carbon footprint than regular cement.

"Production of Portland cement is very bad for the environment because it releases a lot of carbon dioxide into the atmosphere," Nazarian said. "Which of course is something we try to avoid."

Nazarian co-led an interdisciplinary team that earned second place and $466,670.67 in Phases 2 and 3 of NASA's 3D-Printed Habitat Challenge competition between 2017 and 2019. This

Credit: Seana Wood/Penn State

Challenge was established to develop technology necessary to build habitats for future Mars explorers. Along with Nazarian, the team was co-led by José Duarte, the Stuckeman Chair in Design Innovation and director of the Stuckeman Center for Design Computing. Other members of the team included Sven Bilén, professor of engineering design, electrical engineering, and aerospace engineering; Aleksandra Radlinska, associate professor of civil and environmental engineering; Ali Memari, professor of architectural engineering, and the Bernard and Henrietta Hankin Chair in Residential Building Construction; Nicholas Meisel, assistant professor in SEDTAPP; and Randall Bock, assistant research professor in the Department of Agricultural and Biological Engineering.

The team's proposal for the virtual design of the habitat on Mars built on Nazarian's previous research to design innovative material interfaces that would result in the construction of seamless shelters that featured impermeable bonds between the glass and the geopolymer concrete.

"This structure would start at the base with 100% geopolymer concrete made locally with materials that would be sourced on Mars, including basalt rock, kaolinite, sodium, silicon, and ice" Nazarian said. "It would be built such that the glass content would increase reaching 100% where natural light is needed. The concrete would also contain cork within the thickness of the structure, with increasing cork content towards the exterior to provide radiation and thermal protection (referencing functionally graded cork-concrete 3D printing studies with José Duarte). So, this is a great example of a functionally graded structure that could maintain its formal continuity while using functionally graded materials with varying performative characteristics, and where the density and the performative characteristics of the material can change gradually and seamlessly throughout the structure."

The impermeability of the structure would have other benefits for future Mars explorers and mission planners.

"The whole structure becomes impermeable as a unibody if sintered and annealed through the thickness of the structure and across its surface including areas that would allow light in," Nazarian said.

The next step for Nazarian's research is related to artificial intelligence (AI). She and her team are planning to use AI.

"Using AI to develop algorithms would enable us to accomplish precise design, synthesis, and optimization of the distributed constituents in composite and functionally graded materials," Nazarian said. "The use of AI is a necessary step in preparation for 3D printing functionally graded materials. It would enable us to deposit the precise ratio of the constituents in the composite materials in exactly the right place and manage the proper density and properties that we need to engineer and achieve the required performance throughout the structure. This is the next goal I hope to achieve." ■

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