2018

TECHTRACKS

Materials Science and Engineering
A. James Clark School of Engineering

All-Solid-State Batteries: Rapid Li-ion Transport Gives Way to Enhanced Performance

Chair's MESSAGE

Dear MSE Friends and Colleagues,

It has been a very good year for our Department, with a number of very exciting research results in fields ranging from stable, efficient solid state electrolyte design for lithium ion batteries, to the development of modified wood with mechanical properties better than steel, to flash annealing of high entropy multicomponent nanoparticles, to strategies for Perovskite solar cells which can better resist environmental degradation. Our faculty and students published more than 130 articles, an all-time high, in journals including those with the very highest impact: the Nature series, Science, the Advanced Materials series and the Proceedings of the National Academy of Sciences; it was a banner year for invited talks and keynote addresses at professional meetings for us. Our faculty have also shown considerable innovation in the development of new technologies, like the solid state cooling device described in this issue.

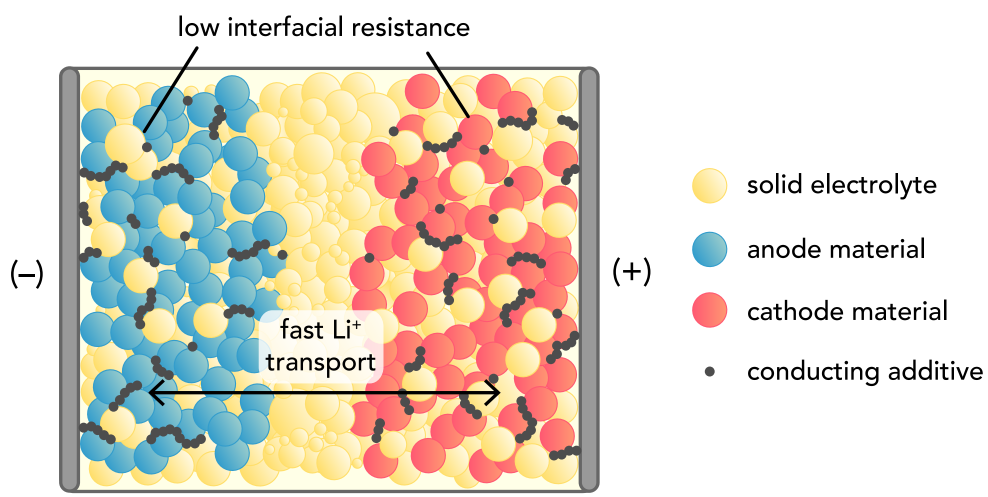
Recognition of their achievements has come through awards at the University, including a Distinguished Scholar Teacher Award, and by selection to senior positions in professional societies. This year saw the launching of the Maryland Energy Innovation Institute (MEI2), and the extension of the DOE Nanostructures for Electrical Energy Storage (NEES) Energy Research Frontiers Center. Our students have been active, not only in research, but in promoting social dialog. We had a very successful review of our undergraduate program by ABET, leading to our reaccreditation for another six years. Our undergraduates continue to excel, with 67% participating in research, with another Capstone Design team going onto a national competition (the Collegiate Inventors finals), multiple students moving onto graduate school at top-ranked institutions, and two of our students winning NSF Graduate Research Fellowships. Our Department reached an all time best ranking, of 24th in the nation according to US News and World Reports. Indeed it has been a very good year.

Raymond J. Phaneuf
Professor and Interim Chair, MSE

IN THIS ISSUE:

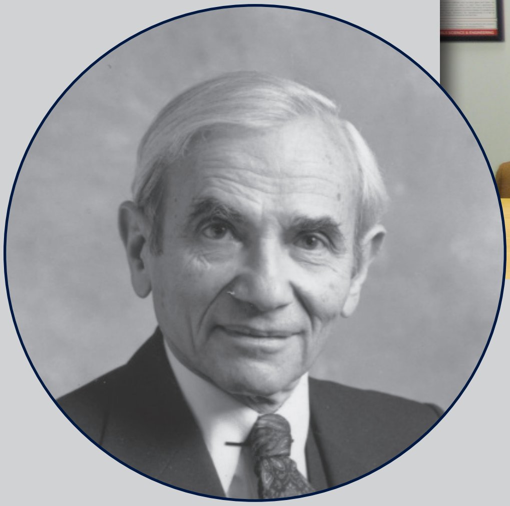
ON THE COVER:

MSE researchers Yiefei Mo and Adelaide Nolan discover new solid electrolyte materials, page 4.



MSE.UMD.EDU | FACEBOOK.COM/MSEUMD | YOUTUBE.COM/MATERIALSATUMD

Prof. Joseph Silverman Honored for His Service to UMD



MSE Professor Emeritus Joseph Silverman (pictured left, and above, bottom left) celebrated his 96th birthday with the Department. Dr. Silverman pioneered the radiation chemistry program at UMD, was part of the team that installed the MUTR TRIGA reactor in 1960, and served as an early director of the Institute for Physical Sciences and Technology.

Photo (left): MSE Team for the 2018 Alumni Cup Competition, hosted by the Clark School of Engineering each spring. This year's team consisted of: Alan Kaplan, Kailey Stracka, Alex Epstein, Alice Tsao, Ricky (Liqi) Zhu, RJ Gins, Shannon Donaldson and Alison Kriz.

For additional information, visit https://eng.umd.edu/alumni-cup-competition. Photo Credit: Jon Consoli for UMD.

COVER**story**

COMPUTATIONAL TECHNIQUE USED TO DEVELOP NEW ALL-SOLID-STATE BATTERY, PUBLISHED IN *JOULE*

Lithium-ion batteries (LIBs) are the most commonly used energy source for household electronics and electric vehicles; however, these LIBs utilize a liquid electrolyte, which has a limited energy density. All-solid-state batteries (ASBs), on the other hand, use a solid electrolyte – an inorganic, non-flammable ceramic material; thus, all-solid-state batteries have the potential to improve upon the energy density, and safety, of current Li-ion batteries.

The development of all-solid-state batteries faces several challenges including a lack of fast Li-ion conducting ceramics, and mechanical and thermodynamic instability between solid ceramic interfaces. However, solid electrolytes and solid interfaces can be studied using computational materials modeling: a powerful tool used to investigate fundamental mechanisms, to predict and discover new materials, and to propose novel engineering strategies for all-solid-state batteries. Computation, for example, can predict new coatings for the interface at the anode, enabling lithium metal anodes, which provide significantly higher energy density than liquid electrolyte counterparts.

In the most recent issue of *Joule,* Materials Science and Engineering (MSE) Assistant Professor, **Yifei Mo**, and his research group were invited to review state-of-the-art computational modeling techniques - for example, *ab initio* molecular dynamics (AIMD) simulations and thermodynamic calculations - and their application in the design of materials and interfaces for all-solid-state Li-ion batteries.

The review focuses on the unique contributions of computation to fundamental scientific understanding of solid-state battery materials at the atomic scale. Computation can predict the detailed dynamics of each individual atom on a femtosecond timescale (one thousandth of trillionth of a second).

"With computation, we can directly observe the diffusion mechanisms of lithium ions, which was impossible before," said **Adelaide Nolan**, a MSE Ph.D. student and first author on the review. "Through these techniques, for the first time, we understand why some solid materials are fast ion conductors, which are critical to achieve high power in solid-state batteries."

This understanding also laid the foundation for the discovery of new solid electrolyte materials with improved performance. First-principles computation is based on fundamental physical principles, allowing scientists to make predictions about new materials with no empirical input.

"The conventional way to develop new materials is very time consuming," said Mo. "By using predictive quantum mechanical calculations combined with supercomputers, we can significantly accelerate the development of new battery materials such as solid electrolytes and electrodes."

Dr. Mo's group is a pioneer in this area – having discovered several new ion-conducting materials – and is working with industry partners to commercialize some of these computationally predicted materials. The research conducted by Mo's group is performed on supercomputers at UMD.

According to the research paper, "these computational studies exemplify the spirit of the MGI [Materials Genome Initiative] in addressing materials problems and in accelerating the design and discovery of new materials for ASBs. Moreover, these computational approaches are also applicable in the study of materials and interfaces in new technologies other than solid-state batteries. However, major research efforts are still required to achieve a comprehensive set of design principles for fast ion conductors."

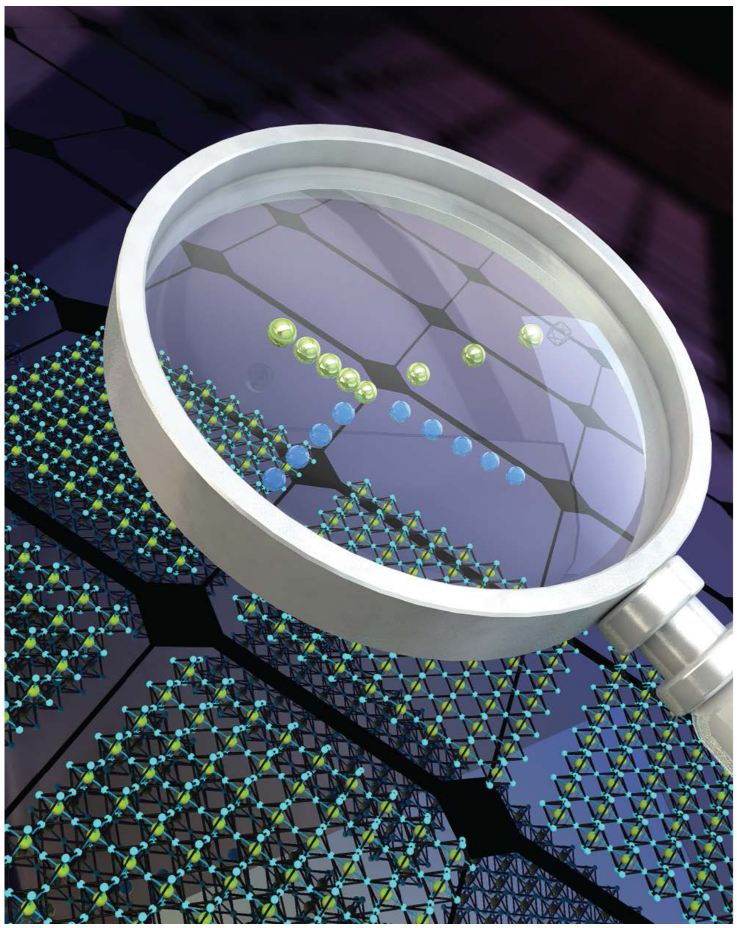
For additional information:

Nolan, A.M., Zhu, Y., He, X., Bai, Q., Mo, Y. Computation-Accelerated Design of Materials and Interfaces for All-Solid-State Lithium-Ion Batteries. Joule, 20 Sept 2018.
DOI: 10.1016/j.joule.2018.08.017.

Leite Group Defines Perovskite ‘Humidity Loop’

Perovskites - a relatively new class of photovoltaic materials developed for use in solar cells – offer a highly efficient and cheap method for converting sunlight into usable energy, but they are also sensitive to ambient conditions, often degrading under exposure to light, water, oxygen and high temperature. Understanding how and why these materials react the way they do under various environmental conditions is critical to the future development of affordable solar technology, and could help mitigate the consequences of global warming.

Researchers in the Leite Lab at the University of Maryland (UMD) use state-of-the-art microscopy techniques to study solar materials and determine how their structure, processing, and performance are connected. In their latest study, **Marina Leite** – an assistant professor in the UMD Department of Materials Science and Engineering (MSE) - and her team identified the impact of the environment on perovskite materials. This study was recently published in the Journal of Physical Chemistry Letters. **John Howard**, an MSE graduate student and UMERC Fellow, served as first author on the paper.



To understand the physical and chemical processes that lead to degradation, the Leite Group exposed these materials to various environmental factors in the lab and measured their response. According to the study, the team used a technique called “in situ environmental photoluminescence (PL) to temporally and spectrally resolve the light emission within a loop of critical relative humidity (rH) levels.”

“We found that the humidity pathway determines the overall optical response of the perovskite materials, leading to a behavior called luminescence hysteresis, wherein the light emitted from the material depends not only on the current conditions but also the prior ones,” said Howard. “Further, we found that the amount of luminescence hysteresis is highly dependent on the ratio between two critical elements constituting the perovskites: Cs and Br.”

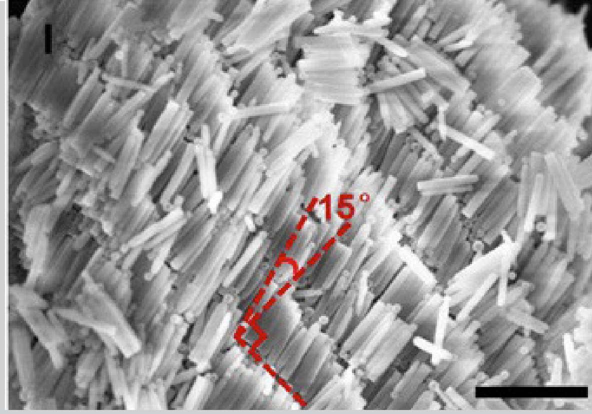
If the moisture-tolerance of the cells can be controlled, or improved, it could give way to a new generation of solar cell technology, which is the Group’s ultimate goal. Moreover, they are working to expand their measurement capabilities on degradation parameters, focusing specifically on temperature.

“For many compositions, the desired perovskite phase becomes unstable at 85 °C, a temperature required for PV stability testing in a number of countries, including the U.S.,” said Howard. “We would like to combine temperature with various humidity and oxygen conditions to measure the combined effect, which is even closer to the real-world conditions these materials would face once commercialized.”

For additional information:

Howard, J.M., Tennyson, E.M., Barik, S., Szostak, R., Waks, E., Toney, M.F., Nogueira, A.F., Neves, B., and Leite, M.S. Humidity-Induced Photoluminescence Hysteresis in Variable Cs/Br Ratio Hybrid Perovskites. *The Journal of Physical Chemistry Letters*, Oct 2018, 9 (12), 3463-3469. **DOI: 10.1021/acs.jpclett.8b01357.**

Liquid crystal material created from particles



Scientists in the University of Maryland (UMD) Departments of Materials Science and Engineering (MSE) and Chemistry and Biochemistry (CHEM) have discovered a new type of liquid crystal (LC) based on particles of inorganic materials, abundant on Earth. The group focused their efforts on exploiting the LC behaviors of particles that have the shapes of organic LC molecules, in order to develop cheaper and more efficient LC materials. This study was published in *Science Advances* on May 11.

The three primary types of LCs, or mesophases, are nematic, smectic and cholesteric. Cholesteric - often called the chiral nematic phase - changes color when exposed to various temperatures, which is why it's commonly used in thermometers, inks and paints.

The molecules of traditional LCs – being anisotropic – take the form of a disc or rod. The shape of the molecule, in part, affects the 'arrangement' that the LCs settle in. Straight, rod-shaped LCs – typically used in flat panel televisions – have been studied extensively for almost a century. Bent-core (i.e., banana-shaped) LCs, discovered roughly 20 years back, can exhibit rich new mesophases, distinct from traditional straight, rod-shaped LCs and show promise in the use of electro-optical devices and light shutters.

What's unique about this study is the use of bent rod-like colloidal particles to reproduce the LC behaviors of banana-shaped molecules. Compared with molecular LCs, colloid-based LCs are thermally stable, cheap and more sensitive to external fields, making them attractive in applications ranging from sensors to displays and metamaterials.

Imagine you toss a fairly large box of pencils onto a desk. Depending on the strength of the toss, the pencils will end up pointing in (roughly) the same direction. "Strength" represents an external field, such as temperature, or an electric or magnetic field.

To make the 'pencils' easier to manipulate and align, "it's best to use colloidal materials, which have a gelatinous texture, for liquid crystals" said **Yang Yang**, a MSE/CHEM post-doc and first author on the study. "When the shape of rod-like particles is curved rather than straight, the rods align in a more complex manner, depending on their geometry," (e.g., bending angles, aspect ratios and bending position).

Colloids - like Jello, Mayonnaise or toothpaste - are somewhere between a solid and a liquid. They can be more stable than small molecules or polymers and not as temperature-sensitive, making them more efficient. There are situations when liquid crystals made of small organic molecules or polymers serve as scaffolding to give the colloids structure. The advantage of the colloids fabricated by this group is that they can adopt their own structures.

Dr. Yang's rods only take a few hours to grow are made of silica, which is basically beach sand – the most common mineral on Earth - meaning they're inexpensive to produce. When the rods slowly settled from a 30-day suspension in DMSO (dimethyl sulfoxide), they positioned themselves to form different ordered LC structures. The organization of rods was characterized by scanning electron microscope (SEM) and polarized optical microscopy (POM). A theoretical model was developed to confirm and predict the LC behaviors of bent rods.

"You can use electric fields to orient them, which offers variations in color and transparency," said Dr. Yang. Although these rods are achiral in nature, they can pack in a chiral manner to maximize a system's efficiency.

"This can give rise to ferroelectric behavior, which requires a lower electric field to make the molecules change direction," said **Luz Martínez-Miranda**, a MSE professor and co-author on the study, .

"We can make large enough quantities to continue studies like this," said MSE professor **Isabel Lloyd**, another co-author. "In other techniques, you don't have enough rods to even think about organizing them. This method could have dental applications, too. This is one step in the process of being able to mimic the microstructure of what your teeth look like under a microscope, in a polymer composite."

Lloyd added, "This is a fundamental study that will lead to bigger and better things, and even more applications."

For additional information:

Yang, Y., Pei, H., Chen, G., Webb, K., Martinez-Miranda, L., Lloyd, I., Lu, Z., Liu, K., Nie, Z. "Phase behaviors of colloidal analogs of bent-core liquid crystals." *Science Advances*, May 2018. **DOI: 10.1126/sciadv.aas8829**

Takeuchi's Group Develops Compact Solid-State Cooling Device

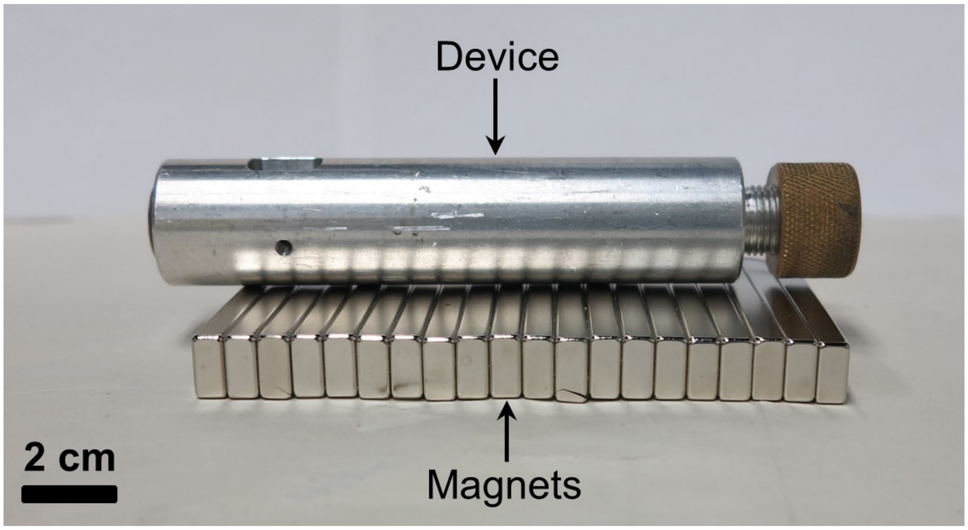
A research team in the UMD Department of Materials Science and Engineering (MSE) has developed a novel compact solid-state cooling device, which can be used to prevent household electronics - such as laptops - from heating up, or even to treat epilepsy via local cooling of the human brain.

'Caloric cooling' is an emerging field of 'green cooling,' which is making current refrigeration technology, via vapor compression, obsolete. Vapor compression uses chemical refrigerants, which are environmentally hazardous, whereas caloric cooling, uses high-efficiency, solid-state cooling materials. Two types of caloric cooling are magnetocaloric and elastocaloric, which use magnetic fields and mechanical stress (~150 MPa in this case) to induce cooling in various materials.

Until recently, caloric cooling technology - though 'green' and efficient - still boasted numerous challenges, delaying widespread commercialization. Magnetocaloric cooling materials, for example, require very large magnetic fields, which can only be supplied by expensive, permanent magnets. Likewise, existing elastocaloric materials suffer from the requirement of hefty mechanical force.

MSE Professor, **Ichiro Takeuchi,** and his group have developed a new kind of composite caloric device, which combines the magnetocaloric and elastocaloric effects. A temperature change as large as 4K can be generated with 0.16 Tesla; more than a factor of 10 lower than the level required for typical magnetocaloric materials.

"By integrating a magnetostrictive material called Terfenol-D and a Cu-based shape memory alloy, we are able to demonstrate ultra-low-field magnetic-field induced cooling for the first time," said Takeuchi. "Due to its unique mechanism arising from a composite effect, we call it the magneto-elastocaloric effect."



Terfenol-D is a mixture of iron - which is very rigid - and terbium - which is so soft it can be cut with a knife. Mixing of the two elements into TbFe2 creates a magnetic function, so that Terfenol-D is responsive to magnetic fields.

"The Terfenol-D extends when a magnetic field is applied to it, and retracts upon removal of the magnetic field, a property called magnetostriction," Takeuchi explained. "Adding dysprosium to the original formulation lowers the required amplitude of magnetic field, which is attractive for transduction technologies."

Magnetostrictive technology is used to build actuators and sensors, such as underwater sonar and energy harvesting devices. In gadgets - portable sound systems, for example - magnetostriction is used for sound wave compression.

The device will look like a hand-held gadget, similar in size to a flashlight. Together with its auxiliary components, the device will be portable, easy-to-use, inexpensive and boast broad application. "Because our composite device is naturally compact, we believe it will open up new cooling applications for caloric cooling, which had not been possible before," said **Huilong Hou**, a post-doctoral researcher in Materials Science and Engineering at UMD and first author on the study.

For additional information: Hou, H., Finkel, P., Staruch, M., Cui, J., Takeuchi, I. "Ultra-low-field magneto-elastocaloric cooling in a multiferroic composite device," *Nature Communications*, Oct 2018. **DOI: 10.1038/s41467-018-06626-y.**

Takeuchi Receives UMD Distinguished Scholar-Teacher

MSE Professor, **Ichiro Takeuchi**, received the University of Maryland's Distinguished Scholar-Teacher Award for the 2018-2019 acadmic year (photo above: Provost **Mary Ann Rankin**, Takeuchi, and President **Wallace Loh**; credit: Stephanie S. Cordle for UMD). The Distinguished Scholar-Teacher Program honors a small number of faculty members each year who have demonstrated notable success in both scholarship and teaching.

Takeuchi – who received his Ph.D. from UMD in 1996 and joined the faculty in 1999 – has helped to reshape the identity of the MSE Department. He's recognized in the research community for having pioneered the combinatorial approach, allowing synthesis and screening of a large number of different compounds in order to rapidly discover new materials. This 'approach' is recognized as one of the main pillars of the Materials Genome Initiative, launched by President Obama's administration in 2011. Takeuchi has participated in a number of workshops and panels on the initiative hosted by the White House. His versatile style of research has led to several discoveries, including the invention of electrostatic cooling, an alternative non-vapor compression cooling technology, which won the UMD Invention of the Year Award in 2010. In line with his award, Takeuchi gave a presentation entitled, "Robot (Materials) Science: Can Watson Beat Edison?" on November 1.

Takeuchi also received the A. James Clark School Outstanding Research Award for his invention of thermoelastic cooling and sustained leadership in high-throughput materials science over the years.

Wachsman Elected Vice President of ECS

Eric Wachsman - MSE Professor, Director of the Maryland Energy Innovation Institute (MEI2) and William L. Crentz Centennial Chair in Energy - has been elected to the office of Vice-President of the Electrochemical Society (ECS) for a three-year term which began in May 2018. At the conclusion of the three year mark, Wachsman will become ECS President, while simultaneously serving as Chair of the Board of Directors and Executive Committee.

"Electrochemistry is fundamental to the scientific and technological advancements in energy storage and conversion being developed at our campus and around the world, and it is truly an honor that my peers entrusted me in this election to help lead this international society as we address some of society's greatest challenges" said Wachsman.

Dr. Wachsman joined ECS as a graduate student in 1989 and quickly became active in the Society. He currently chairs the Interdisciplinary Science and Technology Subcommittee and the National Capitol Section, and serves on the Board of Directors, Technical Affairs Committee, and Symposium Planning Subcommittee. Wachsman has contributed extensively to the next generation of electrochemists having advised and supervised numerous undergraduate and graduate students, postdocs and research scientists, and mentored several junior faculty. His involvement with students includes founding and serving as faculty advisor for ECS Student Chapters at both the University of Florida and the University of Maryland, with the Maryland chapter winning Outstanding ECS Student Chapter Awards in 2013 and 2017, and ECS Student Chapter of Excellence in 2014, 2015 and 2016.

His research is focused on solid ion-conducting materials and electrocatalysts, including the development of solid oxide fuel cells and electrolysis cells, solid-state batteries, ion-transport membranes, and solid-state gas sensors, with over 250 publications and 20 patents.

Student Group EVE Offers Clark School a Unique Platform

Last fall, MSE Ph.D. Students **Naila Al-Hasan** and **Zoey Warecki** created Empowering Voices in Engineering (EVE), a committee and series of workshops designed to encourage dialogue on campus with the ultimate goal of creating a more diverse and inclusive environment. The initiative was a response to the murder of Richard Collins III - a black student and an Army lieutenant at Bowie State University - who was killed on the UMD campus (by a white UMD student, originally an engineering major) on May 20, 2017.

"The idea began with a focus on having conversations within our Department of Materials Science and Engineering, but we quickly realized we needed to expand," said Warecki.

Over the last year, facilitated workshop themes have included discussions on how to conduct meaningful conversations about race; understanding the meaning of racism and building effective communities to counter the phenomenon, as well as tools and resources available on campus to help UMD community members deal with conflict and trauma.

The spring workshop, which took place on April 11, discussed strategies for moving forward as a community, and outlined specific steps that people can take to bring about collective action. Workshops encourage open and frank discussions on the various themes faced by engineering students, faculty and staff members, but everyone on campus is welcome to attend.

Al-Hasan and Warecki were honored at a ceremony on May 18th for their contributions to the Clark School of Engineering. EVE meets the first Friday of every month in EGR 1110.

NAILA AL-HASAN SPEAKING AT THE MAY '18 WORKSHOP. PHOTO CREDIT: AL SANTOS FOR UMD.

ZOEY WARECKI AND ADVISOR MSE ASSOC PROF JOHN CUMMINGS.

MSE Alum Parag Banerjee asks: How will you impact society?

PHOTO COURTESY OF THE UNIVERSITY OF CENTRAL FLORIDA.

Parag Banerjee (PhD, 2011) knew at a young age that he would one day be a problem-solver – science runs in the family.

"My father was a physicist who developed electron microscopes," he said. "I watched him spend long hours working, at home and in his lab. From our dad, my brother – who is also a physicist – I learned a strong work ethic, in addition to a love of science."

Banerjee arrived at Washington State University from Chandigarh, India, in 1998. After completing his master's in materials science and engineering, he took a job at Micron Technology Corporation in Boise, Idaho. An excellent opportunity to put theory into practice, he learned a lot at Micron, but kept his sites on earning a doctoral degree. While looking into the top programs in the U.S., Parag connected with MSE Professor **Gary Rubloff**.

"Gary and I had a long conversation and I was immediately struck over our commonalities, especially his growing interest in atomic layer deposition at the time," said Parag. An offer was made not long after, and during the summer of 2006, Banerjee began his Ph.D. research at UMD. At the time, he was interested in research that had social relevance and would make an immediate impact on society.

"The Clark School is highly interdisciplinary, and there are so many cross-collaborations going on between departments – it's a very vibrant atmosphere," he said. "The best part of my experience at UMD was the research facilities. Going in, I knew how to formulate a research plan, but not so much on how to implement it – UMD made it easy to execute my plans. Plus, I made some great friends in Professor Rubloff's research group – we all remain close to this day."

Rubloff describes Banerjee as a "stroke of luck" for the group, experienced at a high level on arrival, innovative and persistent. "Parag's talents and dedication made research a splash - nanostructured capacity arrays published in *Nature Nanotechnology* - that set the stage for our 11-year run as a DOE Energy Frontier Research Center. His subsequent thesis work was an indicator of his continuing research excellence," said Rubloff.

In addition to his on-campus studies, Banerjee branched out and spent four months in 2009 at the University of Pennsylvania, under the tutelage of Professor Dawn Bonnell, currently the Vice Provost for Research at Penn.

"Working under Dr. Bonnell was a fantastic experience in that I was tasked with solving completely different problems," said Parag. "I made some good connections there and even published a paper, so I highly recommend collaboration – internships specifically – to current engineering students. It's an excellent way to expand your knowledge."

Currently, Banerjee serves as an MSE Associate Professor at the University of Central Florida. His research interests include atomic layer deposition and etching; surface engineering for catalysis and solar energy harvesting. He is also part of the energy conversion and propulsion faculty cluster.

Banerjee recently made headlines after he and his research partner, Srikanth Singamaneni – a professor in the School of Engineering and Applied Science at Washington University in St. Louis – landed an NSF grant to develop an early warning device for would-be heart attack patients.

"Detection that happens at the molecular level using plasmonics is all optical based," he said. "My Co-PI does everything through spectroscopic techniques, so our idea is to convert optical signals into an electric current, which can be integrated on a chip or on an iPhone, for example. Moving from optics to electric-based systems is where the challenge and innovation is, so we're hoping to make a significant impact."

Parag's advice for current engineering students? "Manage your time well – this is the most important aspect of graduate student life. Aim for a *life* experience, not just academics – it's important to make good friends along the way. Topics studied in engineering are complex – learning them doesn't come easy to everyone - so don't be ashamed to ask for help. Finally, ask yourself what drove you to this profession in the first place and, after you graduate, how do you want to impact society?"

When asked if he hopes to pass on his love of science to his two daughters, Parag said, "I hope I can pass my love of creative pursuits to them! Whatever they choose, I just want them to be happy, confident adults. As a parent, that's about the best we can hope for."

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Techtracks is published for alumni and friends of the Department of Materials Science Engineering at the University of Maryland. Your news and comments are welcome! Please send them to mse@umd.edu.