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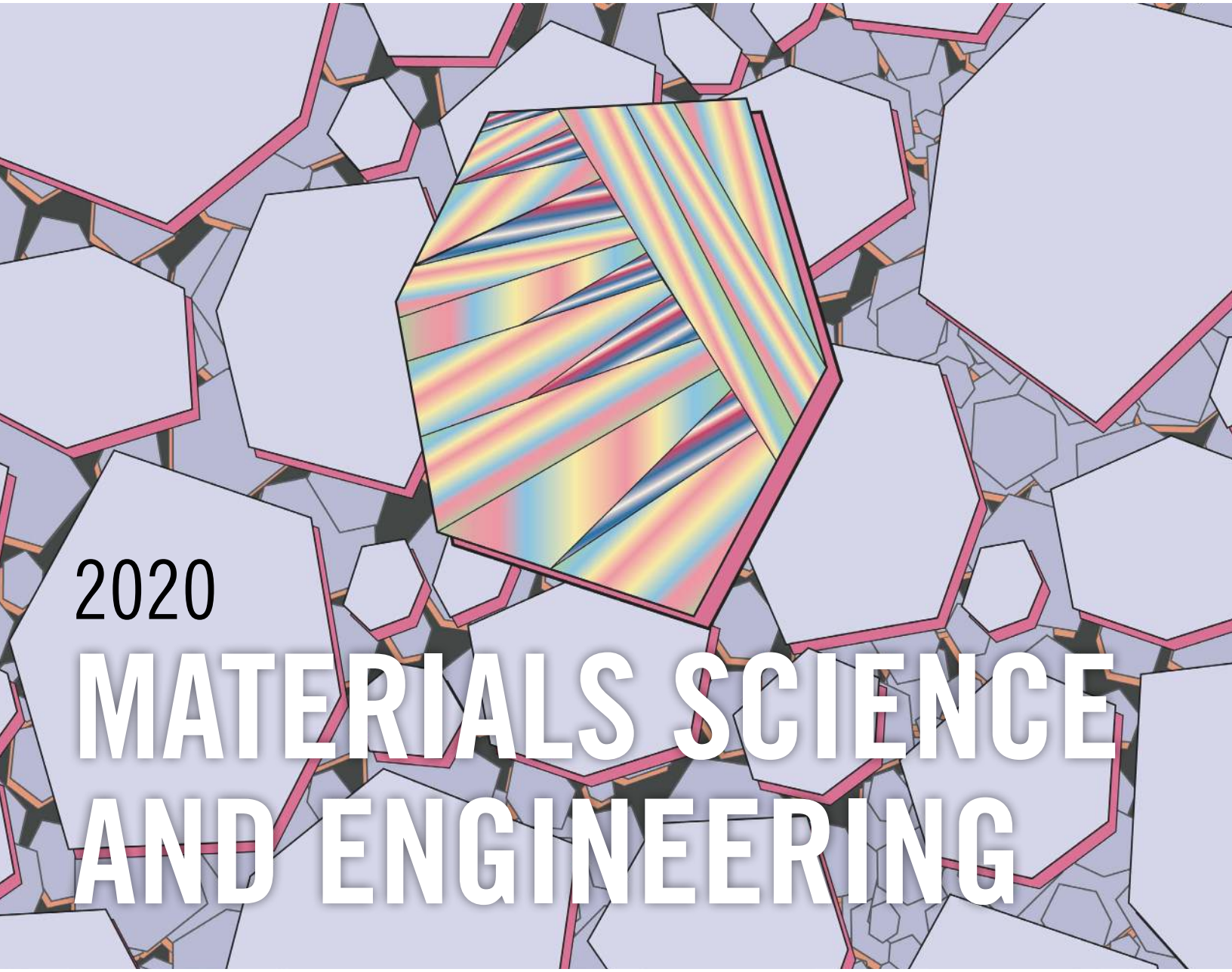


2020 MATERIALS SCIENCE AND ENGINEERING

Pawel Keblinski

Professor and Department Head
Materials Science and
Engineering Department
Rensselaer Polytechnic Institute

WELCOME LETTER

Greetings to our MSE alumni and friends,

The last academic year was dominated by the ongoing COVID-19 epidemic. As a department, we were facing the need to transition to fully online course instruction which was commenced after the spring break and continued through the summer ARCH semester.

WELCOME LETTER

I am happy to share with you that despite this challenge we, including faculty, staff, and students, stepped up to the challenge and, in some cases, we were able to do things even better.

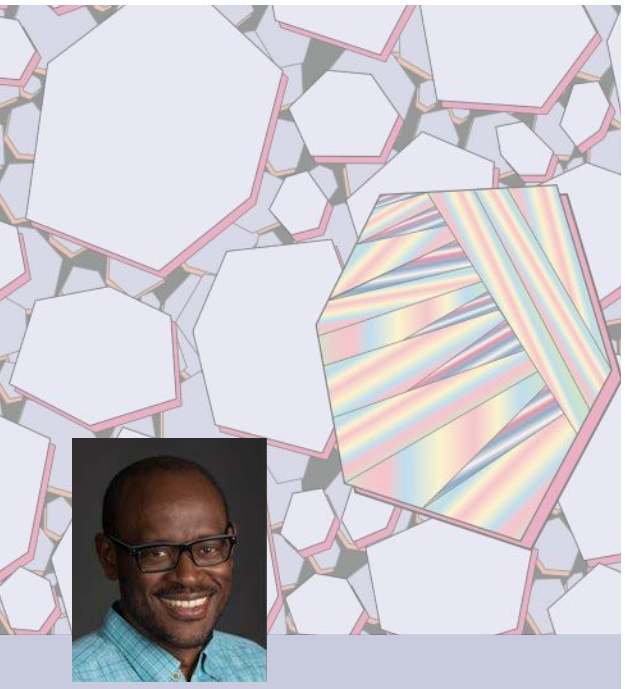
One of our major undertakings was to rearrange our curriculum to minimize the COVID impact. Our summer 2020 ARCH semester coursework focused on the role of theory/computation and analytical tools in materials science and engineering, proving an alternative preparation for Semester Away experience in the fall. Currently, we are working hard on hybrid delivery of fall semester courses. These are simultaneously offered to on-campus and online students, balancing the need of social distancing with the need of practical laboratory experience. In addition, we are focused on maintaining social/professional development activities and interactions via online tools and forums.

In this installment of the MSE News, you will find highlights of our recent achievements and new developments within the MSE community at RPI. Among the highlights are several recognitions of our faculty, most prominently Professor Ravishankar Sundararaman's AIME (American Institute of Mining Engineers) Robert Lansing Hardy Award (2020). This award recognizes an early career scientist in metallurgy and materials science each year, and was awarded to Professor Sundararaman for "seminal contributions to transmute and harness quantum electronic structure calculations for computational materials design in diverse fields of materials research including electrochemistry and plasmonics." The last and only RPI recipient of this award, before Professor Sundararaman, was George Ansell in 1961. George Ansell was perhaps the most successful Dean of Engineering at RPI, and later became president of the Colorado School of Mines.

In this issue of the MSE News, you will also find many other compelling stories. Professor Chaitanya Ullal was recognized for his excellence in research and education with a promotion to the rank of an associate professor with tenure. Professor Edmund Palermo used his expertise with anti-bacterial coatings to anti-viral applications to realize COVID-19-related funding opportunities and design self-sterilizing masks, while Professor Jian Shi demonstrated how to exploit dislocations in halide perovskites for more efficient light-to-electrons energy conversion. Finally, join me in congratulations to a number of our graduate and undergraduate students for their achievements, distinctions, and service, and in welcoming our newest staff member, Ericka Johnson, who will focus on helping the administration of our graduate program.

Please enjoy the stories we report to you and share any thoughts, ideas, and your own successes with us.

Thank you,
Pawel Keblinski



On the Cover: Professor Edwin Fohtung's research group recently published an article in Advanced Electronic Materials, which focused on using X-ray nanovision to capture *in situ* nanoscale phase transformations in a single BaTiO3 nanocrystal.

GRADUATING CLASS OF 2020

We are enormously proud of our graduating seniors and co-terminal master's degree recipients who completed their degrees in the midst of a pandemic. They are bound for careers in industry and for further studies in graduate school. Congratulations and we wish you the very best of luck!

A few of our graduating students are pictured below in a socially distanced manner. We hope to celebrate with all of you in person at some time in the future!

Chunyin Yang

Mimi Williams

Nicholas Hoffman

Arun Baskaran

Alex Perkins

Dante Boyd

Matthew LaBranche

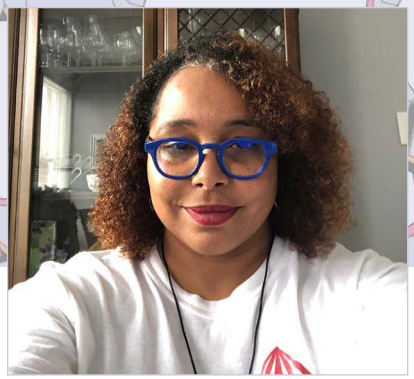
Liv Williams

Sarah Dalakos

Zhuoqun Wen

Hanchuan Yang

Priyanka Mehta



STAFF SPOTLIGHT

Ericka Johnson joins the front office staff. Welcome!

Hi, my name is Ericka Johnson and I am the Administrative Specialist for the Materials Science & Engineering Graduate Program Administrator. I recently moved back to the New York area from Colorado, where I lived for the past 20 years. I grew up in New York City, where I attended grade school and high school. I then earned a B.S. in Psychology from Union College in Schenectady, New York. I also attended The Culinary Institute of America in Hyde Park, N.Y. and obtained an associates degree in the culinary arts. Right after culinary school I moved to Aspen, Colorado, and worked in various restaurants and catering establishments as an executive chef. I came to RPI in December 2019 and have enjoyed working at RPI and being back in upstate New York. The staff, faculty and students have been very helpful and welcoming, making my time here thus far an easy transition.

FACULTY NEWS

Professor Jian Shi Appointed Associate Editor of Journal of Applied Physics

Professor Jian Shi is now an associate editor for the Journal of Applied Physics. Dr. Shi has previously served as an early career member in the Editorial Advisory Board of JAP. In his new role at the prestigious journal, Dr. Shi will be mainly handling manuscripts on "Dielectrics, Ferroelectrics, and Multiferroics." Dr. Shi's research covers strain engineering, symmetry engineering, and neuromorphic computing.

Recently, Dr. Shi has been also selected as this year's recipient of the James M. Tien '66 Early Career Award at RPI! This award honors early career achievement in research and teaching. More information about Professor Jian Shi's outstanding work can be found here: http://homepages.rpi.edu/~shij4/index.html

Professor Liping Huang selected fellow of the American Ceramics Society

Professor Liping Huang has been selected to become a fellow of the American Ceramics Society (ACerS). The fellow designation recognizes ACerS members who have distinguished themselves through outstanding contributions to the ceramic arts or sciences, broad and productive scholarship in ceramic science and technology, conspicuous achievement in ceramic industry, or by outstanding service to the Society.

ACerS recognized the importance of Professor Huang's work with the citation: "Dr. Liping Huang has achieved international recognition for the fundamental understanding she brings to the atomic structure and mechanical behavior of amorphous materials from combining experimental techniques such as in-situ Brillouin and Raman spectroscopy with computational approaches."

Professor Pawel Keblinski Named MRS Fellow

Professor Pawel Keblinski was named a 2020 Materials Research Society fellow. The Materials Research Society (MRS) fellows program recognizes outstanding contributions to the field, including research, leadership, and service that have advanced the mission of the materials community world-wide. It is a lifetime recognition of distinction in the field, capped at no more than 0.2% of the MRS membership in any given year.

Professor Keblinski joined RPI and the Materials Science and Engineering (MSE) Department over 20 years ago, and he currently serves at the Department Head. His research relies mainly on the use of classical molecular dynamics simulations to study structure-property relationships in interfacial materials, with a focus on thermal transport modeling. MRS recognized the importance of his work with a fellowship "for influential contributions to the development of computational methods leading to fundamental understanding of thermal transport in materials on nanometer-length scales." Keblinski's work to date has resulted in over 200 publications in peer-reviewed journals, and over 23,000 citations, and an associated H-index of 66 (Google Scholar). He is also a Humboldt Fellow (Germany), Marie Curie Fellow (EU Commission/Poland), and a fellow of the American Physical Society.

Professor Sundararaman Receives AIME Robert Lansing Hardy Award

Ravishankar Sundararaman, an assistant professor in the Materials Science and Engineering Department at Rensselaer, has been selected as the 2020 recipient of the AIME Robert Lansing Hardy Award from TMS.

The Hardy Award recognizes a young person in the broad fields of metallurgy and materials science for exceptional promise of a successful career. Ravishankar will receive the award at the TMS Annual Meeting in San Diego on February 26, 2020.

FOUNDER'S AWARD OF EXCELLENCE

Congratulations to four of our outstanding materials students, Dante Boyd, Zhizhong Chen, Zhuoqun Wen, and Matthew H. LaBranche, who are among the recipients of the 2019 Founders Award of Excellence. Established in 1994, the Founders Award "honors students who embody qualities of creativity, discovery, leadership, and the values of pride and responsibility at Rensselaer." The award consists of a special certificate and a cash prize.

Dante Boyd, a senior and a summer undergraduate researcher in Prof Chaitanya Ullal's group, plans to remain at RPI as a coterminal master's degree in materials engineering, following his graduation in May.

He has been a member of the RPI Men's Soccer Team for all four years of college, including the 2019 season in which the team set records for total wins, win streak, and an unbeaten streak, as well as hosting the Liberty League Tournament and advancing to the Sweet 16 of the NCAA Tournament, both for the first time in school history. He was selected to the Liberty League All-Academic Team all four seasons. Prior, Dante has also received the Arthur Ashe Jr. Sports-Scholar Award (2019).

Zhizhong Chen, a graduate student advised by Professor Jian Shi, focuses his research on understanding the relationship between the symmetry of novel perovskite-related materials and their electronic and dielectric properties. He has authored and co-authored more than 10 papers on this topic, including such top-tier journals as *Advanced Materials*, *Science Advances*, and *Nature Communications*. He has also mentored and influenced three undergraduate students who were URP students in the past and are currently pursuing their Ph.D. degrees in other universities.

Zhuoqun Wen, a senior and an undergraduate researcher in Professor Jian Shi's group, did research on developing a novel growth method for low-dimensional and phase transition materials. He has been in the Shi group for two semesters and has made various contributions in his research projects. Starting in 2020, he will pursue his Ph.D. in materials science and engineering at the University of Michigan – Ann Arbor.

Matthew LaBranche, a senior in Professor Yunfeng Shi's group, has performed cutting-edge research on chemically and mechanically strengthened glasses through molecular dynamics simulations. Besides being a Rensselaer Medalist, he was also selected to be a Corning Scholar and has presented his work to Corning Research Fellows in the spring 2018 semester. He has served as the Captain of the varsity men's soccer team since his sophomore year. Under his leadership, the team attained Sweet 16 status in the NCAA Tournament. He will join W.L. Gore and Associates as an engineer after, and hopes to specialize in new product development.

Ullal Promoted to Associate Professor with Tenure

Professor Chaitanya Ullal joined the Materials Science and Engineering faculty at RPI as an assistant professor in 2013. Recently, he was promoted to the rank of associate professor with tenure, a richly deserved achievement. Dr. Ullal earned his Ph.D. in materials science and engineering at MIT and did a post-doc in the lab of Professor Stefan Hell (Nobel Prize in Chemistry, 2014), at the MPI-BPC in Goettingen, Germany. He is a recipient of an NSF CAREER Award and an ACS PRF New Investigator Award. This past year, Professor Ullal was awarded the 2020 Eastern NY Alfred H. Geisler Memorial Award that recognizes an outstanding young materials scientist/engineer from the Eastern NY ASM chapter who has made significant contributions in the fields of education, research, or manufacturing.

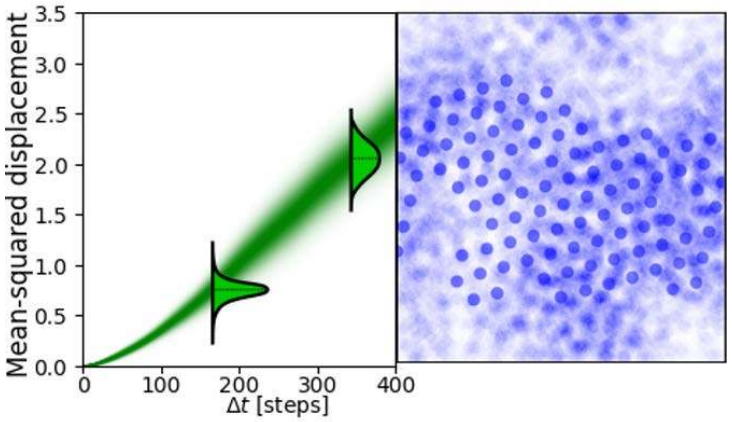
Dr. Ullal's research interests are related to polymers, unconventional nanolithography, and optics. A current emphasis of his work is the imaging and patterning of 3-D nanostructured polymers via super-resolution optics, which circumvents the diffraction barrier and achieves nanoscale resolutions while using visible light and far-field optics. Over the course of his career so far, Dr. Ullal has published 39 peer-reviewed articles in top-tier journals such as *Advanced Materials*, *Nature Materials*, and *Chemistry of Materials*. This body of scholarship has been recognized with more than two thousand citations and an h-index of 21. His research has been funded my multiple major grants from the National Science Foundation, as well as Industrial grants.

UNDERGRADUATE CURRICULUM COMMITTEE

MTLE Summer Arch 2020 Goes Virtual with Fully Redesigned Curriculum

The Materials Engineering Department has rapidly responded to student concerns over the ARCH Summer 2020 semester, to be delivered via remote instruction amid the COVID-19 pandemic. Members of the Undergraduate Curriculum Committee (UCC), along with the Department Head Professor Pawel Keblinski and the relevant faculty instructors, have met with the MTLE class of '22 to discuss their concerns and priorities moving forward. The faculty actively engaged with students to understand their perspectives and adjusted our curriculum accordingly.

Previously, the summer session was utilized for lab-intensive course work geared towards engineering proficiency in an industrial setting. Now, the department has reoriented the summer curriculum towards courses that emphasize equally important skill sets: things like data dexterity, modeling, simulations, and engineering math techniques. For this summer 2020, a materials-centric version of Modeling and Analysis of Uncertainty (MAU, our core statistics course), will be delivered jointly by Profs. Keblinski and Sundararaman. Professor Ozisik will deliver a redesigned version of our Thermodynamics course using virtual laboratories and computer simulations, which are particularly well-suited for such a math-intensive course. Professor Dan Lewis will pioneer a new focused course, Math Skills for MTLE, which will give students the tools to efficiently process and analyze data sets and to perform industry-relevant calculations. Taken



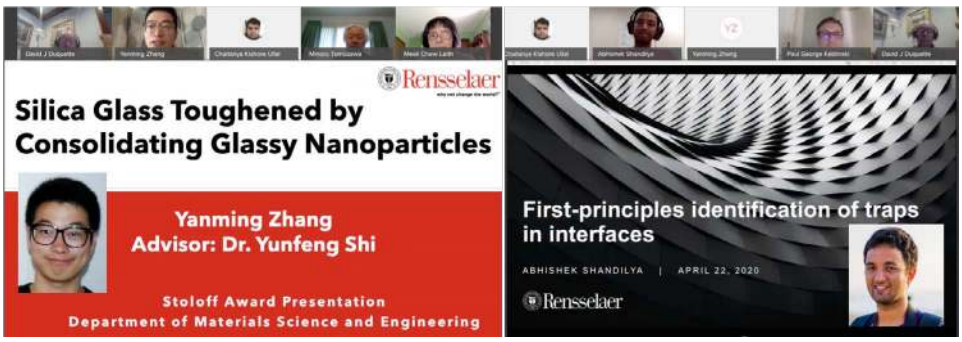
together, these three courses will equip our students with a firm foundation of computational know-how, which will be ideally suited for a time when face-to-face and hands-on learning have been temporarily paused. The laboratory-intensive courses that have been replaced this summer will now be offered in the spring and fall 2021 semesters.

Despite the difficulties presented by the unparalleled COVID-19 public health crisis, RPI Materials Engineering students are well-positioned to enhance their computational skills during the 2020 academic year. We wish them all the very best and are looking forward to working with them in the semesters to come.

GRAD STUDENT NEWS – STOLOFF AWARD

Congratulations to Yanming Zhang (Y. Shi group) and Abhishek Shandilya (Sundararaman group) for winning this year's Norman S. Stoloff Research Excellence Award! This award is to recognize MSE graduate students for their outstanding research accomplishments, as evidenced by a submitted or published journal article in the past 12 months. This award is presented annually to up to two current MSE graduate students. Recipients will receive a cash prize and a certificate of the achievement. The winners presented a virtual talk/ webinar as part of the department seminar series.

Yanming's article in Nano Letters is titled "Silica Glass Toughened by Consolidation of Glassy Nanoparticles" and Abhishek's article in Journal of Materials Research is entitled "First-principles identification of localized trap states in polymer nanocomposite interfaces." We are so proud of you both for these fine accomplishments!



Material Advantage

Material Advantage is our student-run MTLE organization for professional development, outreach, and social events. Members attended the TMS conference in February 2020 (pictured). We also did an afterschool outreach program in nearby Watervliet, with the Engineering Ambassadors club, as well as participating in Exploring Engineering Day.

Our most recent Election Results are in! President: Ky Lamarca, VP: Gia Trzaska, Treasurer: Sumati Rangaraj, Secretary: Sydney Neuman, Publicity Director: Lauren Evans, Outreach Chair: Ryan Hawks

RESEARCH FOCUS

Antiviral Polymer Coatings on Self-Sterilizing Facemasks

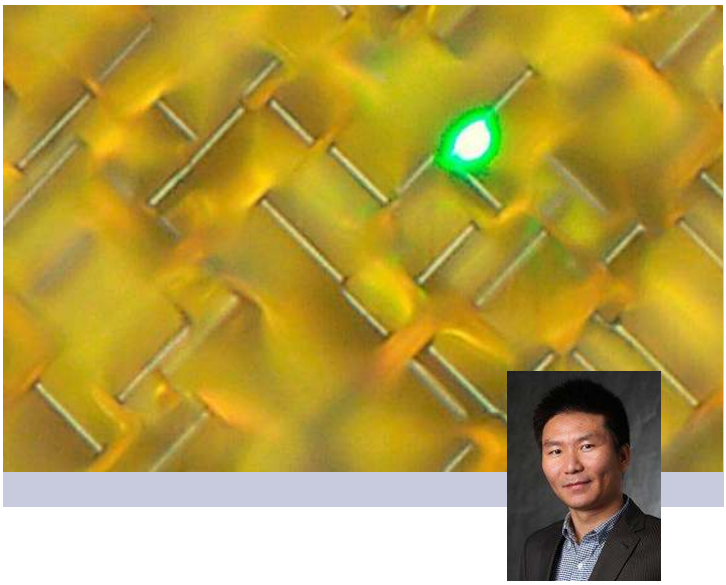
Assistant Professors Helen Zha (Chemical Engineering) and Ed Palermo (Materials Science) have teamed up to develop a method for coating fibrous filter materials — such as melt-blown polypropylene microfibers found in N95 facepiece respirators — with actively antiviral surface properties. This effort could lead to personal protective equipment that actively eliminates virus on contact. With $200k in support from a newly awarded National Science Foundation Rapid Response Research (RAPID) grant, the researchers plan to examine ways to equip N95 respirator masks with antiviral properties. These improvements would better protect health care workers and enable the current supply of masks to last longer.

N95 masks are designed using very small electrostatically charged fibers that help prevent aerosolized droplets of the virus from penetrating through the mask material. The design, while effective, doesn't lend itself to disinfection and reuse, further exacerbating the effects of a limited supply. "N95s are designed to be taken off and thrown away immediately after you've seen a patient," said Zha. "The idea we have in mind is to develop a process where someone in the hospital can apply a very thin coating of an inexpensive polymer material to the mask stock that they already have, that will give it antiviral properties and also enable sterilization procedures." Palermo adds, "Our proposed technology would make the mask self-disinfect by inactivating viral particles on contact. Such a technology could enable health care workers to safely use the same mask for longer periods of time."

Zha's expertise in making ultrathin protein and polymer coatings on surfaces, combined with Palermo's expertise in antimicrobial polymers, form an ideal partnership for this research effort. Once their research is complete, Zha and Palermo will work with a team at Mount Sinai to deploy this coating in order to confirm its feasibility in a hospital setting. The team will then share its findings with other researchers and the public through open accessible channels.

"For our frontline health care workers, access to PPE is a matter of life and death," Congressman Paul Tonko (D, NY-20) said. "This project, developed by the incredible minds at Rensselaer Polytechnic Institute, takes essential steps to address the shortage of these materials, which will save precious lives in our Capital Region and beyond."

Role of Dislocations in Halide Perovskites Unveiled



A promising semiconductor material could be improved if flaws previously thought irrelevant to performance are reduced, according to research published in *Nature Communications*. Professor Jian Shi of the MSE department at RPI led the effort with researchers from several other universities. They have shown that a specific defect impacts the ability of halide perovskite to hold energy derived from light in the form of electrons.

Research on halide perovskite has rapidly improved the efficiency of the material from about a 3% conversion of light to electrical energy to 25% — equivalent to state-of-the-art silicon solar cells — over the course of a decade. Researchers wrestled with silicon for decades to reach that material's current level of efficiency.

Halide perovskite also has promising carrier dynamics, which are roughly defined as the length of time that light energy absorbed by the material is retained in the form of an excited electron. To make a good prospect for solar energy conversion, electrons in the material must retain their energy long enough to be harvested by an electrode attached to the material, thus completing the conversion of light to electrical energy. The material had long been considered "defect tolerant," meaning flaws like missing atoms, shoddy bonds across grains of the crystal, and a mismatch known as crystallographic dislocation were not believed to have much impact on efficiency. More recent research has questioned that assumption and found that some defects do affect aspects of the crystal's performance.

Shi's team tested whether the defect of crystallographic dislocation impacts carrier dynamics by growing the crystal on two different substrates. One substrate had a strong interaction with the halide perovskite as it was being deposited, producing a higher density of dislocations. The other had a weaker interaction and produced a lower density of dislocations. The results show that dislocations negatively impact the carrier dynamics of halide perovskite. Reducing dislocation densities by more than one order of magnitude is found to lead to an increase of electron lifetime by four times.

The research was supported by grants from the National Science Foundation and the Air Force Office of Scientific Research.

RENSSELAER IN THE NEWS

RPI Researcher Uses Simple Formula For Chemical Reactions To Predict COVID-19 Trajectory

A scientist at Rensselaer Polytechnic Institute has created a coronavirus transmission model inspired by one he uses to predict chemical reactions to help the Centers for Disease Control and Prevention forecast COVID-19 deaths across the country.

Developed by Yunfeng Shi, an associate professor of materials science and engineering at Rensselaer, and Jeff Ban, a professor of civil engineering at the University of Washington, the model uses fatality data collected by Johns Hopkins University and mobility data collected by Google to predict disease spread based on how much a population is moving within its community.

The researchers tested their model against data from 20 of the hardest hit counties in the United States and found it to be valid. Their findings are available in preprint on medRxiv, an online repository of papers that have been screened but not peer-reviewed.

The team has also been able to show how the forecasts change as schools open, communities lockdown and masks are mandated. The researchers' website, which illustrates those forecasts, was developed by Tanooj Shah, a graduate student in Shi's group.

"There's no mystery as to why there's an outbreak," Shi said. "There's no mystery to how we control it. The science is absolutely there. We want to use the model to give the local government some concrete predictive insight to implement certain policies."

Shi is a computational materials scientist who was curious about how simple chemical reaction analogs could be applied to forecasting COVID-19 transmission. Combined with Ban's expertise in transportation and mobility, the two have developed a straightforward model that has been accurately predicting disease transmission.

They are now sharing their unique approach to forecasting COVID-19 spread with the CDC on a weekly basis, along with a collective of other research teams made up of infectious disease specialists, machine learning experts and modelers from across the nation. Combined, the models form an ensemble forecast from a multitude of perspectives.

"The novelty of the model lies in the integration of physical modeling and data-driven approaches, which can bring useful insights about the infection and outbreak of COVID-19," Ban said. "The findings of the research, such as the critical relative mobility indicator, can be used by policymakers for making informed decisions about when and how to reopen local economies."

The engineers plan to continue sharing their model results each week for the duration of the pandemic.

Pawel Keblinksi, the head of the Department of Materials Science and Engineering at Rensselaer, said the model is unique because of its simplicity and that it demonstrates that social mobility is a major contributing factor in controlling the spread of the virus.

"This is an example of 'the minimalist' approach that Professor Shi used successfully to model complex physical reactive processes, including polymer or complex crystal growth," Keblinski said.

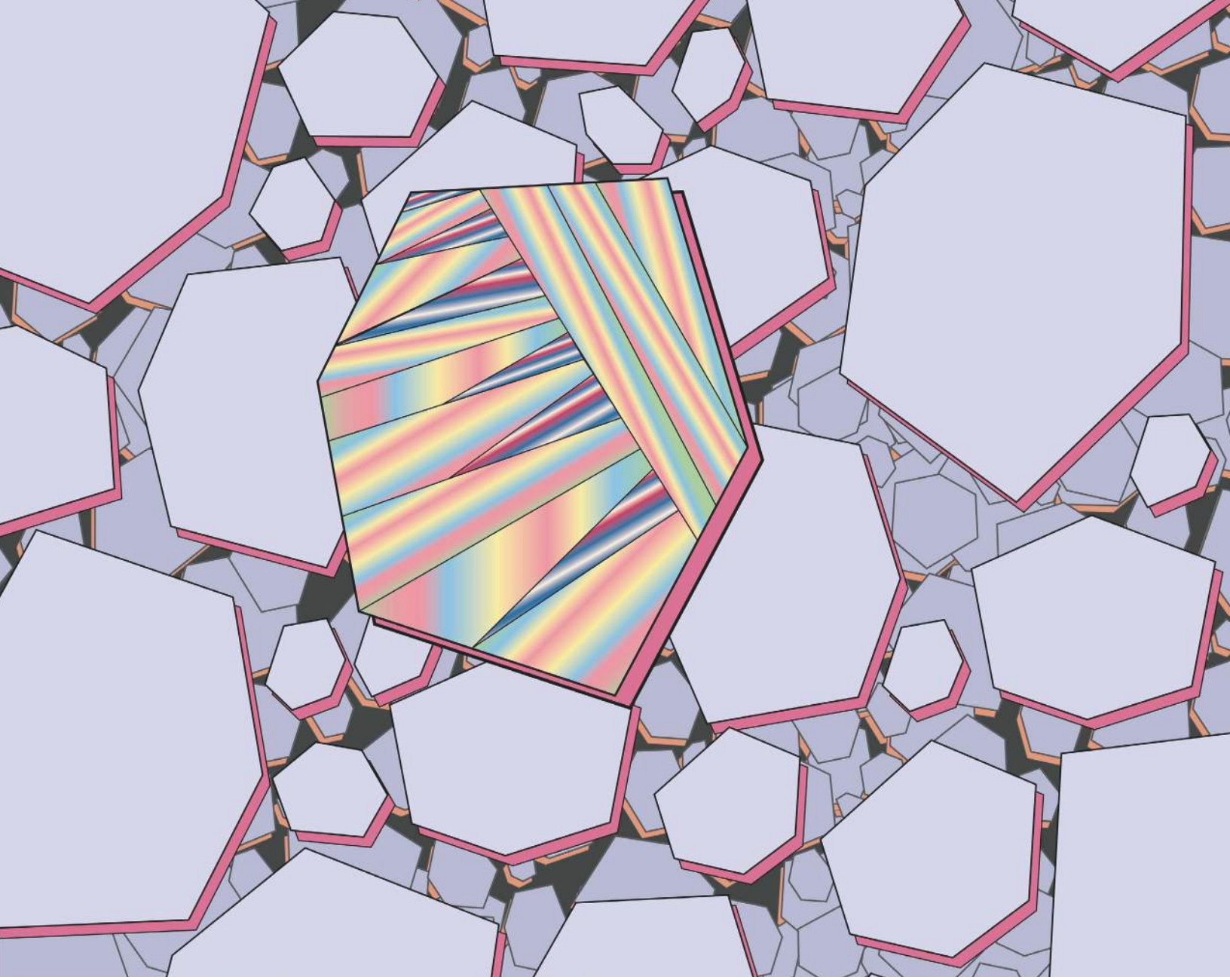
This article originally appeared in the Albany Times Union, Oct. 22, 2020.

Screenshot of the visualization of our model on a website developed by Tanooj Sha, a first-year MSE graduate student.

"The idea to model infectious disease transmission as a chemical reaction analog is not new. What enables this work is the availability of mobility data from Google that can be incorporated into a compartment model straightforwardly. From the point of view of a molecular modeler, atoms are much more friendly to understand than humans. To this end, when we first processed COVID-19 data and saw an almost straight line, it was indeed a pleasant surprise."

Yunfeng Shi

Associate Professor, Materials Science and Engineering



WE WANT TO HEAR FROM YOU!

Please let us know what you are currently doing so we can include you in future newsletters. If you know of any MS&E alumni/ae who have not received this newsletter, please send us their names and addresses and we will add them to our mailing list.

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