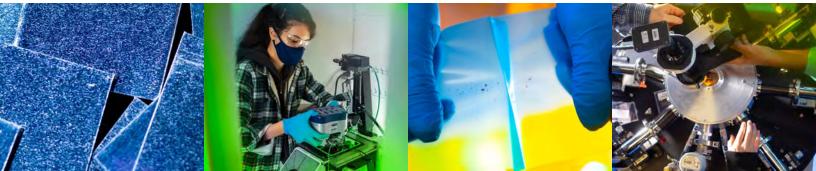


University at Buffalo Department of Materials Design and Innovation

School of Engineering and Applied Sciences College of Arts and Sciences

LEADING THE WAY

EXTRAORDINARY GROWTH IN 2021 POWERED BY THE STRENGTH OF OUR FACULTY AND STUDENTS



Chair's Welcome



Erich Bloch Chair, SUNY Distinguished Professor and Empire Innovation Professor

Department of Materials Design and Innovation

Dear Friends,

A year ago, in the inaugural edition of FACETS, I had written that "... we are witnessing a surge of problems in all aspects of our lives – climate change, emerging diseases, ... and ... their seriousness and urgency demand solutions ... that can accelerate scientific discovery and problem-solving abilities so that we can work faster and smarter."

Little did I know that those words would unfortunately become prophetic as we face an unprecedented pandemic. This has, as it has for everyone, been a time that tests our resilience both individually as well as collectively as a community. At this point of reflection in the young history of our department, I can say how fortunate I feel to be part of the MDI family. As will be elaborated on in this issue of FACETS, the accomplishments in the department reflect the strength of its faculty and students.

Our faculty continue to garner national recognition for their research and educational excellence through NSF CAREER awards and SUNY Distinguished Professorships. Two of our faculty successfully gained promotions to the Associate level and were granted tenure. International recognitions to our graduate students through best paper awards and professional society awards reaffirmed the stature of our young department.

This past year marked critical renewals of two of our major multi-million dollar center efforts, the NSF Science & Technology Center - BioXFEL and the Collaboratory for a Regenerative Economy (CoRE). These programs reflect the unique nature of our research portfolio in MDI, advancing science at the nexus of information science, experiments, and modeling, to unique applications of materials science.

MDI continues to be in a leadership position in UB's School of Engineering and Applied Sciences in receiving external research grants and graduating PhD and MS students. We are proud that another seven new PhDs have joined the ranks of our alumni. They continue to be impressive ambassadors for MDI as they get hired at national labs, leading industrial labs and top ranked universities.

The Erich Bloch Symposium was revived after a year break and held virtually to a large national audience. We adapted to the pandemic environment and embarked on our NSF REU program, by hosting it in a virtual fashion.

This year marked the growth of new external partnerships such as the MDI-Brookhaven National Laboratory (BNL) joint agreement that establishes joint appointments between MDI faculty and BNL. This now creates new opportunities for closer collaboration between our groups, the first of its kind between BNL and UB.

With the establishment of a highly successful graduate program, we are proud to welcome the first class of undergraduate students enrolled in MDI to join us, delayed by a year due to the pandemic.

Finally, despite the challenges of the last year and a half, we are at the next point of our department growth as we recruit four new faculty members over the next one to two years. Speaking of the future, we are privileged to announce our MDI Board of Advisors, an internationally distinguished panel of individuals who will help us chart the future of MDI.

And, 2021 marks the retirement of **Margie Poniatowski**, MDI's Administrative Director. Margie has guided the building and operation of the department from its very inception. Since 2015, she has facilitated and guided all aspects of the administrative activities in MDI. She has been the sounding post, and patient advisor to faculty and students alike. For me personally, I could not have undertaken the task of building this department without her help. It is with mixed feelings I see Margie leave for her next phase of activities after her extraordinary years of service to UB and especially to MDI. I know I speak on behalf of all the students and faculty in our department when I say a heartfelt thank you and best wishes for the future.

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MDI at a Glance

2021 By the Numbers

FIRST SET OF STUDENTS ENROLLED IN UNDERGRADUATE COURSES

3:1 graduate student to faculty ratio

10 STUDENTS PARTICIPATED IN THE FIRST YEAR OF NSF REU PROGRAM ON DATA DRIVEN MATERIALS DESIGN

13 FULL-TIME FACULTY AND GROWING RECRUITING FOUR FACULTY TO JOIN MDI OVER THE NEXT 2 YEARS

\$250,000-\$300,000 AVERAGE RESEARCH EXPENDITURES PER FACULTY

OVER \$6 MILLION FROM INDUSTRY AND PRIVATE FOUNDATION INVESTMENTS Enrollment: Fall 2021

2 undergraduate students

6 MASTER'S STUDENTS

21 PHD STUDENTS

Graduation: 2020-2021

MASTER'S STUDENTS

PHD STUDENTS

MDI Board of Advisors



Frank Alexander

Deputy Director, Computational Science Initiative, Brookhaven National Laboratory



Raymondo Arroyare

Professor, Department of Materials Science, Texas A&M University



Tammie Borders

Senior Business Development Manager, Honeywell Quantum Systems



Sheila Davis Director, Silicon Valley Toxics Coalition



William Harris

Chair, MDI Board of Advisors, CEO, Arizona Science Foundation



Carl Kesselman

Dean's Professor, University of Southern California Viterbi School of Engineering



Benji Muryama

Autonomous Research Lead, Materials and Manufacturing Directorate, Air Force Research Lab



Susan Sinnott

Chair, Department of Materials Science and Engineering, Penn State University

Meet our Faculty



Bill Bauer ASSISTANT PROFESSOR

OF RESEARCH

I manage MDI's Research Experience for Undergraduates (REU) program, which trains a diverse group of undergraduate students in the interdisciplinary skills needed to employ a data-driven approach to the design of new materials. I also manage the education and diversity programs for UB's Science and Technology Center (STC), BioXFEL. Through the STC and REU, I have incorporated underserved students into STEM fields at UB, the Hauptman-Woodward Institute (HWI) and other sites across the country. I was born and raised in Buffalo and started working as an intern at HWI while a junior in college. I received a PhD in Structural Biology from UB and now run the same internship program that I started in. I have found that working with students and helping them to realize their full potential has been very gratifying.



Scott Broderick ASSOCIATE PROFESSOR OF RESEARCH

My research improves the performance and characteristics of materials across a broad range of applications. For example, my research has societal impact by making structural materials stronger and tougher, preventing corrosion and delaying the failure of materials used in corrosive environments, making battery lifetimes longer, improving the efficiency of nanomedicines, and reducing the use of toxic elements without compromising performance. These results are achieved through the integration of traditional materials science with data science, thereby demonstrating the power of the MDI approach for the future of materials. As data becomes more widely available, the ability to harness all of that information is critical. My work in developing computational tools leads to understanding, visualizing and utilizing complex data, with the tools made available to the community, thereby expanding their impact. I became interested in materials science in high school, and as an undergrad saw the need for focusing on a broader design perspective. My hometown is Apex, North Carolina.

Baishakhi Mazumder

ASSISTANT PROFESSOR

My research establishes comprehensive understandings of structure-chemistry and atomic-scale phenomena that impact the materials system with an overarching goal of improved material properties and functionalities for a wide range of applications. For example, enhancing the performance of ultra-wide bandgap materials relies on a critical understanding of mechanisms to efficiently generate and control charge carriers and how these carriers interact within the materials. The outcome of this research can improve power conversion efficiency in a variety of applications including consumer appliances, all-electric and hybrid-electric vehicles, and extraction and conversion of cost-effective renewable energy sources. This in return will save energy, significantly reducing costs, benefiting both the economy and environment. Our research approach is to integrate advanced materials and property characterization methods with machine learning modeling and establish a direct link with the material functionalities that would be difficult to achieve otherwise. I am from Kolkata, West Bengal, India.

Prathima Nalam ASSISTANT PROFESSOR

My research focuses on tuning material properties by modifying their surface and interface. Careful design and modification of the top few nanometers to micrometers of any surface will provide desired properties to any engineering material. This also helps improve the performance and service life of engineering parts and components. My lab focuses on developing fundamental understanding in interfacial science and mechanics to develop surfaces that present low friction and are also resistant to degradation and wear. There is a constant need to develop novel materials through interface engineering, either to enhance engine efficiencies or tackle novel and less-detectable toxins. This calls for a research approach that combines advanced interfacial characterization with computational methods. This approach, when coupled with machine learning methods, accelerates both material selection and selection of interfacial design strategies. Hence, the paradigm shift in our approach to interfacial engineering advances the MDI vision very well. I come from Vishakhapatnam, a warm coastal city in South India.



Erik Einarsson ASSOCIATE PROFESSOR

I work primarily on graphene, which is a single atomic layer of carbon with a wide range of impressive properties. In particular, the unique electrical properties of graphene make it amenable to operation at very high frequencies. My research is focused on terahertz frequency antenna arrays, which couple electrons in graphene to free-space electromagnetic waves. This technology will enable next generation 6G wireless communications, and the underlying science will reveal materials properties in the least explored portion of the electromagnetic spectrum. I became interested in this area when I moved to UB and wanted to combine my background in carbon nanomaterials with the emerging field of terahertz spectroscopy. The broad range of energies and length scales involved in this interdisciplinary research is a great fit to MDI. I grew up in Columbia Falls, Montana, and came to UB from the University of Tokyo in 2013.



Quanxi Iia

SUNY DISTINGUISHED PROFESSOR, NATIONAL GRID PROFESSOR DF MATERIALS RESEARCH, AND EMPIRE INNOVATION PROFESSOR

My research is centered on the processing-structureproperty-performance relationship of nanostructured and multifunctional materials and devices which have found wide applications in microelectronics, energy, and information technologies. Over the years, I have worked on the forefront of materials research to answer such scientific auestions as how can we push the limits of syntheses to create materials with improved and emergent properties and how can functionalities of materials be tuned by defects, interface, and heterogeneity. The broader impact of my innovations and discoveries is documented through the issuance of 50 U.S. patents and publication of over 500 peer-reviewed journal articles. My work augments MDI's goal to address society's need for acceleration of design and discovery of new materials that impact a broad range of technological applications. I was born to a family of six children in a small village in Henan Province, China.

Bruce Pitman

I develop statistical methodologies to accelerate materials discovery. One of my current interests is in developing statistical emulators, which are fast approximations that estimate the result of complex and time-consuming computational or physical experiments, based on training data. Importantly, these emulators come equipped with an error estimate. That is, the emulator predicts what the result of an experiment would have been, had it been run, and the range of likely outcomes. This probabilistic feature is a key ingredient in uncertainty quantification. Most recently I have been studying emulators of functional outputs - an experimental output that is a function of space and/or time. These statistics-based methods are one part of a larger effort directed toward explainable machine learning. Because these emulator methods are probabilistic in nature, the results let the user judge how confident to be with those outcomes. That can, in turn, inform the subsequent use of the results. I grew up in New Jersey, but have lived in Amherst, New York, for over 30 years.



Krishna Rajan

ERICH BLOCH CHAIR, SUNY DISTINGUISHED PROFESSOR, AND EMPIRE INNOVATION PROFESSOR

My initial work was motivated by exploring data intensive imaging and trying to develop new ways of integrating multiscale information from the subsequent data. These methods were based on tools used in the field of data mining and my interest in using these methods for other forms of data initiated my efforts into the broader field of what I call 'Materials Informatics'. Informatics is the 'third leg' – along with experiments and computation – in materials science. Because the role of Materials Informatics is pervasive across all aspects of materials science and engineering, its impact is pervasive across many disciplines. I feel privileged to have been given the opportunity to establish a new department based on this vision of materials science; allowing us to impact both education and research in addressing pressing social issues. I was raised mostly in Canada but lived in many places around the world before reaching Buffalo six years ago.

Meet our Faculty (continued)



Kristofer Reyes ASSISTANT PROFESSOR

I apply mathematics and machine learning to problems in materials science. I am especially interested in using machine learning meaningfully when there is limited data available to train data-hungry models. We encounter this "smalldata" setting often in materials science. I work on machine learning methods that integrate additional information from simulations, physics models, and domain experts, and build algorithms that intelligently decide the best data to collect. We use these algorithms in autonomous robot scientists in designing materials science experiments, several of which have made discoveries in mechanical structure design, nanomaterials optimization, and flow chemistry. My background is a mix of computational materials science, mathematics, and computer science, and I have industrial experience centered around data and machine learning. I was born in Manila, Philippines, but grew up in Michigan. I went to Purdue University for my undergraduate degree in mathematics and computer science, and the University at Michigan for my PhD in Applied Math. I have also lived/worked in the Washington DC area, NYC and Princeton, NJ.



Jung-Hun Seo ASSISTANT PROFESSOR

My research focuses on the development of inorganic freestanding single crystal semiconductor nanosheets and flexible electronics based on these semiconductor materials. There is a wide spectrum of electronics applications where higher speed (or high power) and mechanical flexibility are simultaneously needed, such as wireless communications, remote sensing and airborne/space surveillance. High-performance flexible electronics consume much less power when operated at a reduced speed, and wirelessly connected devices enabled only by high operation speed/frequency are more convenient to use. Therefore, my research can benefit new fields such as wearable electronics or environmental monitoring systems. My research advances MDI's mission through the way multidisciplinary aspects of knowledge including material science, electrical engineering, physics and mechanical engineering, are systematically studied, to implement various material and device parameters. I am from Seoul, South Korea, and moved to the University of Wisconsin-Madison, where I earned my MS, PhD, and worked as a Postdoc. I came to Buffalo in 2016 to join UB's MDI department.

Eddie Snell PROFESSOR

Proteins are the building blocks of life, enzymes are efficient machines, and life has materials with many unique properties. My work is to explore the structure and function of the building blocks of life, both in static and dynamic states. This knowledge will enable the use of these machines for industrial processes with high efficiency, understanding the nature of disease and treatment, and developing materials that mimic those that makeup living organisms. My current interest is in the metals that biological organisms require and how they achieve the specificity of the needed metal in a metal-rich environment. From a materials perspective, I am interested in the analysis methods and how they impact the observation of the material, and how to correct for that impact. My work advances MDI's mission by bringing sophisticated analysis methods to probe biological materials. My hometown is Liverpool and I completed my PhD in Chemistry at the University of Manchester. I spent a decade at NASA's biophysics laboratory at Marshall Space Flight Center in Alabama before moving to Buffalo where I am also President and CEO of the Hauptman-Woodward Medical Research Institute.

Olga Wodo ASSOCIATE PROFESSOR

My work is centered around microstructure informaticsthe branch of materials science linking information with microstructure science. The methods we develop are foundational for designing high-efficiency solar cells, membranes for water filtrations, and soil remediation-as in all those applications, microstructure controls the device efficiency. We use graphs to effectively capture the key topological and morphological features of the microstructure that are critical for the properties. Our work extracts information from microstructural samples, translates it into a format compatible with modern machine learning tools, and ultimately enables the acceleration of microstructure design for desired properties-the key element of MDI's mission. As a PhD student, I was amazed by the diversity of microstructure materials and at the same time, surprised that many relationships rely on just one microstructural feature - the grain size. The need to expand this feature set has been reaffirmed after joining MDI, where I learned about approaches taken at the atomistic and molecular level. My hometown is Czestochowa, Poland.

Research Highlights

Fei Yao ASSISTANT PROFESSOR

My research interests include two-dimensional materials synthesis, property engineering, and their applications in energy-efficient electrochemical and electronic devices. Research on clean energy holds great promise to mitigate climate change and secure the energy supply. Energy science encompasses a broad range of research areas spanning a variety of applications that involves efficient and clean energy storage, conversion, transport, and utilization. Its development requires interdisciplinary knowledge ranging from the fundamental understanding of the interfacial phenomenon to technology innovation at the device level. We will leverage data science as an efficient toolkit to facilitate the discovery, design, and realization of two-dimensional materials and therefore improve the performance of electrochemical energy storage in advanced batteries/supercapacitors, energy conversion in fuel cells, and energy efficiency in nanoelectronics. I was born in Shandong Province, China, and received dual PhD degrees in Energy Science from Sungkyunkwan University, Korea, and in Physics from Ecole Polytechnique, France, in 2013.

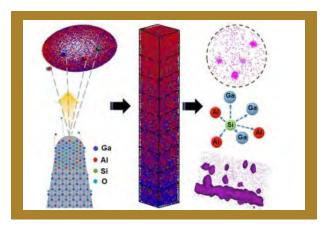
WE'RE HIRING!

MDI has launched its next phase of faculty growth and invites candidates to apply for the positions of Assistant Professor, Associate Professor or Full Professor in four areas: Structural Materials, Computational Materials Science, Microelectronic Materials, and Robotics & Manufacturing in Materials Science.

We are looking for candidates to join a dynamic, interdisciplinary faculty team operating at the convergence of materials science and information science. Successful candidates are expected to work effectively in a novel team environment and integrate well into MDI's innovative teaching and research program. Faculty are expected to teach courses at the graduate and undergraduate levels, mentor graduate students, advise students at all levels and maintain an active research program.

Candidates for an Associate Professor or Full Professor position should have a strong record of scholarly accomplishments, teaching experience and a sustained externally funded research program.

To apply, visit: **engineering.buffalo.edu/home/school/ about/employment.html**



Mazumder wins NSF CAREER award

RESEARCH COULD LEAD TO ENERGY AND COST SAVINGS IN WIDE RANGE OF CONSUMER ELECTRONICS

Materials scientist **Baishakhi Mazumder** received an NSF CAREER award, which will support her research to improve electrical conductivity in ultrawide band gap semiconductors.

Her research has the potential to improve the performance of a wide range of consumer electronics and appliances, all-electric and hybridelectric vehicles, and extraction and conversion of renewable energy sources by saving energy, which significantly reduces costs, and ultimately benefits both the economy and the environment.

"This award reflects Baishakhi's innovative work in atomic scale chemical imaging and its application to addressing fundamental studies in the role of defects in complex materials," says **Krishna Rajan**, SUNY Distinguished Professor and Erich Bloch Chair of MDI.

Mazumder received the \$642,450 award for her project, entitled "Atomic scale understanding of the doping incorporation and transport properties in ultrawide band gap semiconductors," from NSF's Division of Materials Research.

"It is a milestone for MDI to have its first NSF CAREER award winner within the first five years of is inception. Baishakhi's achievement reflects the extraordinary quality of inaugural faculty who are building MDI." —Rajan

Reyes receives joint appointment at Brookhaven National Laboratory

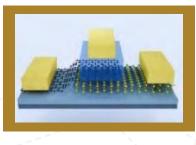
Better drug design, control and learning of materials fabrication processes, and detecting low-dose radiation. These are just a few of the potential issues that **Kristofer Reyes** will tackle as part of his joint appointment with Brookhaven National Laboratory.

Offered by the DOE to researchers who can contribute to Brookhaven's mission at large, the appointment will afford Reyes with the opportunity to collaborate on developing mathematical and machine learning methods for a wide variety of problems.

Reyes is part of Brookhaven's newest directorate, the Computational Science Initiative, which aims to explore all the ways computation, mathematics and machine learning and AI can be leveraged to solve problems of pressing need by the Department of Energy. These include issues in materials design, climate modeling and nuclear non-proliferation.

Atom-thin transistor uses half the voltage of common semiconductors, boosts current density

Fei Yao's work on a new, two-dimensional transistor made of graphene and the compound molybdenum disulfide (MoS2) could have a major impact on quantum computing.



The transistor is composed of a single layer of graphene and a single layer of MoS2, which is a part of a group of compounds known as transition metals chalcogenides. The graphene and MoS2 are stacked together, and the overall thickness of the device is roughly 1 nanometer. While most transistors require 60 millivolts for a decade of change in current, this new device operates at 29 millivolts.

The transistor requires half the voltage of current semiconductors. Another important characteristic is its ability to handle a greater current density compared to conventional transistor technologies based on 2D or 3D channel materials. The transistor can handle 4 microamps per micrometer.

Faculty News

Newly Tenured Faculty

Olga Wodo

ASSOCIATE PROFESSOR

Olga Wodo has established herself as one of the leaders in the field of "microstructural informatics". Process-structureproperty relationships can then be naturally parametrized and explored using this microstructure manifold. The impact of this work is its ability to be adopted to a wide range of materials engineering problems. Researchers in microstructural modeling in materials science describe Wodo's work on microstructure informatics as "one of the most prominent contributions to the scientific community." This demonstrates the caliber of Wodo's work and her reputation as a rising star in the materials science community.

Other Promotions

Scott Broderick

ASSOCIATE PROFESSOR OF RESEARCH

Scott Broderick has created new paradigms in engineering alloy design that has attracted the attention of industry and government agencies. He has developed machine learning aided methods that actually guide the selection of new chemistries that can meet a complex array of engineering requirements that cannot be predicted with classical theories of alloy design. This work has created, for the first time, the concept of a "Periodic Table for Alloy Design." His peers have called his work as providing a "paradigm-changing concept" in significantly accelerating the discovery of new compositions for engineering alloy design.

Jia named SUNY Distinguished Professor

Quanxi Jia was one of five University at Buffalo faculty to be named a SUNY Distinguished Professor, the highest rank in the SUNY system.

According to SUNY, "this distinction is attained through extraordinary contributions to, and impact on, the candidate's field of study, often evidenced by significant research and/or creative activity. The work must be of such character that it has the potential to elevate the standards of scholarship or creative activity of colleagues, both within and beyond their academic fields."

Jia is an internationally recognized leader in multifunctional and nanostructured materials for energy and electronic-device applications. He has authored or co-authored more than 500 peerreviewed journal articles, delivered more than 100 invited lectures and holds 50 U.S. patents.

He is an elected fellow of the American Association for the Advancement of Science (AAAS), National Academy of Inventors (NAI), American Ceramic Society (ACerS), the American Physical Society (APS), the Institute of Electrical and Electronics Engineers (IEEE), the Materials Research Society (MRS) and the Los Alamos National Laboratory.

Jia also serves as the scientific director of UB's New York State Center of Excellence in Materials Informatics. He is the founding co-editorin-chief of Materials Research Letters and the principal editor of the Journal of Materials Research.

Mazumder paper is Editor's Pick in Applied Physics Letters

For the second year in a row, Applied Physics Letters selected research by **Baishakhi Mazumder** as its Editor's Pick.

Applied Physics Letters publishes short experimental and theoretical papers related to applications of physics phenomena in all branches of science, engineering, and modern technology. The article, "Nanoscale compositional analysis of wurtzite BAIN thin film using atom probe tomography," was authored by Mazumder and her student, **Jith Sarkar**.

The paper reports on a nanoscale compositional analysis that will be important in the development of emerging ultrawide band gap material, BAIN with a high B content and larger thickness. It has the potential for use in future high-power electronics and optical applications. Nalam appointed to Tribology Letter's Board of Early Career Researcher

Prathima Nalam is one of 25 researchers to join the Board of Early Career Researchers of Tribology Letters.

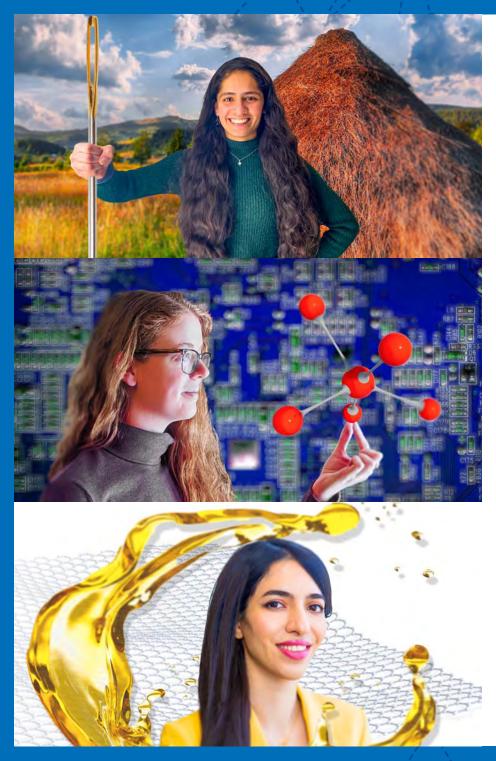
Nalam is primarily interested in developing alternative materials that will leave a lowcarbon footprint on the environment. Her research interests lie in developing next-generation materials in the fields of tribology, filtration, and bioengineering. To achieve this, she employs advanced materials characterization methods, novel functionalization techniques and, if required, couples with machine learning methods to establish structureproperty relationships for novel materials such as 2D materials and biomaterials.

She has published more than 25 peer-reviewed journal publications and is a recipient of the Swiss National Science Foundation Fellowship. She is also an affiliated faculty member of UB's Institute for Research and Education in eNergy Environmental and Water (RENEW).

Student Highlights

Three MDI PhD students among finalists in UB's 3 Minute Thesis competition

ANNUAL COMPETITION CHALLENGES PHD STUDENTS TO SUCCINCTLY AND ENGAGINGLY PRESENT THEIR RESEARCH IN 180 SECONDS WITH JUST ONE POWERPOINT SLIDE



Devyani Jivani presented "Rethinking 'Needle in a Haystack' Approach in Materials Discovery," in which she drew on computational tools to aid the acceleration in prediction of materials' properties based on their microstructure. Advised by **Olga Wodo**, Jivani's research goal is to enable acceleration of materials design and discovery to address the need of environmentally conscious materials with high performance.

Olivia Licata presented her thesis "Design from the Atom Up," advised by **Baishakhi Mazumder**, in which she used atom probe tomography for materials characterization and applied statistical methods for data analysis. The goal of her research is to provide insights that will help improve the design process for semiconductor components.

Behnoosh Sattari Baboukani

presented "Slippery Flatlands." Advised by **Prathima Nalam**, she focused on generating a fundamental understanding of tribological behavior of twodimensional materials to enable them to be used as frictionreducing additives in oil-based lubrication. The goal of her research is to develop novel lubricants for engines using advanced material design approaches.

Students named finalists for International Award

PhD students **Olivia Licata** and **Jith Sarkar** were two of five finalists for the highly competitive international E.W. Müller Outstanding Emerging Scientist Award from the International Field Emission Society (IFES).

Both students are advised by **Baishakhi Mazumder**, a leader in atom probe tomography, and it is the first time that two finalists for the prestigious international award have come from the same advisor.

The award, named after the first man to see an atom, is given to emerging scientists by the IFES. It honors a recent and original work on field emission, field ionization or related phenomena. Participants present their research at the Atom Probe Tomography & Microscopy conference (APT&M), and answer in-depth questions by members of the society and the judging panel.

Zheng receives SEAS Dean's Achievement Award

Yixiong Zheng received the School of Engineering and Applied Sciences Dean's Graduate Achievement Award, which recognizes students for doing exemplary research.



A recent MDI PhD graduate advised by

Jung-Hun Seo, Zheng's research focuses on the synthesis and characterization of various ultrawide bandgap semiconductors. He pioneered a method of heterogeneous integration among nextgeneration ultrawide band gap semiconductors such as diamond and gallium oxide, which are the material building blocks for a myriad of future electronics and optoelectronic applications. He has published eight journal papers, six of which he was first author. He is currently working as a postdoctoral researcher at the University of Wisconsin-Madison.

Events



Erich Bloch Symposium explored how data drives innovation and discovery

WORLD EXPERTS SHOW HOW A DATA-INFORMED COMMUNITY CAN ADDRESS CLIMATE CHANGE, PUBLIC HEALTH AND OTHER PRESSING SOCIETAL CHALLENGES

The "sweet spot" for data-driven science. The growing importance of population data. Online misinformation. Using culture to address climate change. These issues and more were the topics of discussion at the 2021 Erich Bloch Symposium.

The two-day virtual event, which was held on June 7-8, 2021, brought together renowned researchers, policymakers, academics, and industry and community leaders to explore the area of sustainability with a focus on materials, technological innovation, and community health.

The symposium featured nine presentations from a diverse group of scholars whose expertise encompassed astronomy, engineering, geography, art, media and more. Topics centered around the symposium's theme: "The World Through the Lens of Data: Accelerating knowledge discovery in the service of science and society."

The event also included panel discussions from academic and industry leaders, and poster presentations that showcased how MDI students are working to provide solutions to critical societal challenges.

The Erich Bloch Symposium is an annual event organized by MDI. It is dedicated to the late Erich Bloch, a former director of the U.S. National Science Foundation and UB alumnus, who established the Erich Bloch Endowed Chair for MDI in 2014.

The next Erich Bloch Symposium will be held on June 7-8, 2022. Check the MDI website for details.

EPA recognizes MDI work on classifying "forever chemicals"

Forever chemicals are all around us –in many consumer, commercial and industrial products, such as nonstick cookware, stain and water-resistant treatments and takeout containers. Their long-lasting components break down slowly over time. There is much that we don't understand about these chemicals, also known as PFAS (per- and polyfluoroalkyl substances), and their potential negative impacts on the health of humans, animals and our environment.

An important first step in expanding information, transparency and regulation around the thousands of existing PFAS is to develop an effective, efficient system for classifying them. However, due to the large number and diverse types of PFAS, it has been a challenge to develop systematic terminology to describe them.

To help overcome this issue, the Environmental Protection Agency (EPA) announced that they have adopted a computational method developed by MDI researchers **An Su**, a post-doctoral scientist, and **Krishna Rajan**, Erich Bloch Chair and SUNY Distinguished Professor, to build the science driving the regulatory policy of classifying PFAS compounds.

Su and Rajan established a new data framework that links the molecular structural modeling of PFAS chemistry with advanced machine learning tools to rapidly give insight into the fundamental chemistry that drives the classification of PFAS structure and functionality. The details are described in their paper, "A database framework for rapid screening of structure-function relationships in PFAS chemistry," which was recently published in Nature's Scientific Data.

The research will be part of the EPA's National PFAS Testing Strategy, which was established to advance our understanding of PFAS and their impacts.



This work was sponsored by the Collaboratory for a Regenerative Economy (CoRE) directed by Rajan, and the NSF Materials Data Engineering Laboratory project in which Rajan is a co-PI with colleagues in UB's Department of Computer Science and Engineering and MDI.

Connect with MDI



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University at Buffalo Department of Materials Design and Innovation

School of Engineering and Applied Sciences College of Arts and Sciences