# 38th Annual Hilliard Symposium

**May 20, 2021**
**8:20am – 3:40pm CT | ZOOM**

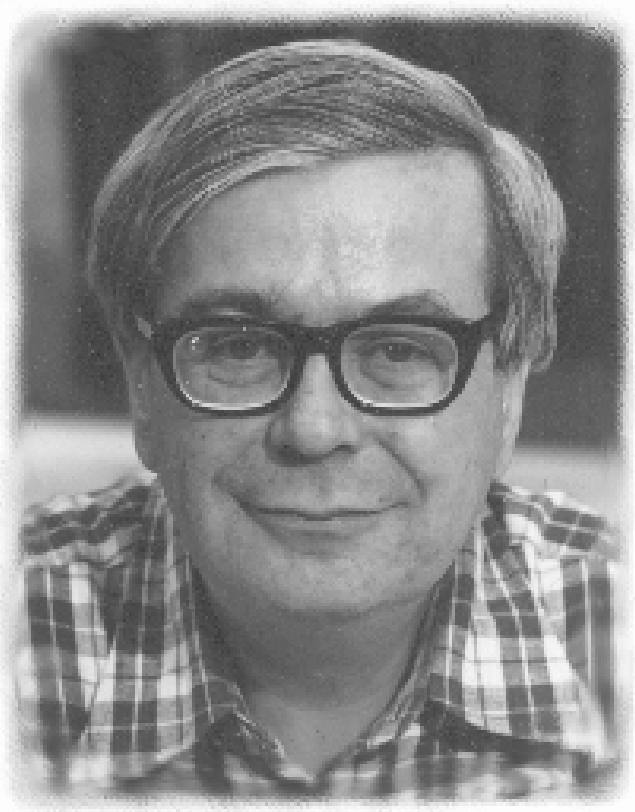
**Winners will be announced at 5:00 pm.**

Artwork by Jack Hegarty, Dravid Group.

# John E. Hilliard, 1926-1987

John E. Hilliard joined the faculty of Northwestern University in 1962 and taught here for the next quarter of a century. Born and educated in the United Kingdom, he received his Ph.D. from the University of Liverpool. There followed a postdoctoral appointment at the Massachusetts Institute of Technology and six years at the General Electric Research Laboratory, before he came to Northwestern.

Dr. Hilliard was an inspiring teacher for not only his students but also for his colleagues and the wider metallurgical community. His work included four areas of research: the study of the thermodynamic and kinetic processes in inhomogeneous systems, the quantitative characterization of structure, the theoretical and experimental study of spinodal decomposition, and the synthesis and investigation of compositionally modulated films. The last two areas represent pioneering work, for which his publications are cited with enormous frequency.



# SPEAKER SCHEDULE

**Central Time Zone**

**8:20 AM** **Welcome by Professor Derk Joester, Symposium Chair**

**8:30 AM** **Keynote by Professor Mariana Bertoni**

**9:30 AM** **Remarks by Professor Derk Joester**

**9:40 AM** **Kristen Wek – Stupp Group, 4th Year**

A Hierarchically Structured Microparticle Platform for Regenerative Medicine

**10:00 AM** **Chase Brisbois – Olvera Group, 5th Year**

Locomotion of Magnetoelastic Membranes

**10:20 AM** **Travis Schmauss – Barnett Group, 5th Year**

Surface Modification of Solid Oxide Electrodes for Robust Energy Storage

**10:40 AM** **Haiyue Huang – Huang Group, 4th Year**

On-mask Chemical Modulation of Respiratory Droplets

**11:00 AM** **10-minute Break**

# SPEAKER SCHEDULE

**11:10 AM** **Raymond Wang – Rondinelli Group, 5th Year**
Learning the Crystal Structure Genome for Property Classification

**11:30 AM** **Luke Prestowitz – Huang Group, 6th Year**
Towards Nanoarchitectonic Materials

**11:50 AM** **Ramya Gurunathan – Snyder Group, 4th Year**
Predicting the Thermal Resistance of Grain Boundaries and Interfaces

**12:10 PM** **James Male – Snyder Group, 4th Year**
Improving Doping in Lead Chalcogenide Thermoelectrics

**12:30 PM** **Diversity, Equity, and Inclusion presentation by Dr. Michael Rawlings, TMS**

# SPEAKER SCHEDULE

**1:30 PM** **Chunyi Huang – Lauhon Group, 5th Year**
Doping Control in Nanowires for Quantum Computing

**1:50 PM** **Sonal Rangnekar – Hersam Group, 5th Year**
An Aerosol-Jet-Printed Graphene Biosensing Platform for Rapid Electrochemical Detection of Proteins and Small Molecules

**2:10 PM** **Allessandra Dicorato – Joester Group, 6th Year**
Multi-Scale Imaging of Nanomaterial-Tissue Interactions

**2:30 PM** **Kelly Parker – Dravid Group, 5th Year**
Soft Microscopy: Advancing High-Throughput Characterization at Low-Voltage

**2:50 PM** **Break**

**3:00 PM** **Donghoon Shin – Mirkin Group, 3rd Year**
Bridging the Gap Between Halide Perovskite Nanocrystals and Thin-Films: Mesoscale Halide Perovskite Arrays

**3:20 PM** **Liban Jibril – Dravid/Mirkin Group, 4th Year**
Nanoparticle Synthesis in Hollow Silica Shell Nanoreactors

**3:40 PM** **Closing Remarks**

# KEYNOTE SPEAKER
# Professor Mariana Bertoni, ASU

**8:30 AM CT**

## Chasing the sun from academia to industry and back again

The solar PV market continues to accelerate in adoption and over the last decade we have seen it move from niche generation to reaching grid parity and becoming a mainstream electricity generation source. The reality of silicon module prices below $\$0.35/W_{dc}$ and updated Nationwide goals of $0.02/kWh by 2030 has fundamentally changed solar R&D. As we move towards an "electric-powered world" and everything around us starts demanding electricity in a clean and efficient way, new challenges arise. Similar to many consumer applications, R&D hurdles centered around aesthetics, customization and functionality will be part of our everyday life.

In this talk, I will share with you my adventures in solar R&D in academia, industry and the start-up world. We will walk through the maturity of various solar technologies, research at the pace of industry and the hurdles for the implementation and mass adoption of new technology.

**Presentation on Diversity, Equity & Inclusion**

**12:30 – 1:30 PM CT**

*Delivered during the Hilliard lunch hour.*

**DR. MICHAEL J. RAWLINGS, TMS**

**Implicit Bias Workshop**

**4:00 – 5:00 PM CT**

*Separate Zoom link.*

**STEFANIE HICKS, NU**

Northwestern | McCORMICK SCHOOL OF ENGINEERING

**Chase A. Brisbois**

B.S., Nanoscale Science, SUNY Albany, 2014

## Locomotion of Magnetoelastic Membranes

Nanoscale magnetoelastic membranes are composites of superparamagnetic nanoparticles that can elastically deform in response to magnetic fields. This class of active material is particularly suited for robotic applications in nanomedicine because they operate at small scales, do not interfere with biochemical systems, and possess no residual magnetization. However, applications in drug delivery or microsurgery necessitate microrobots that swim through their environment. Swimming is challenging at small scales and requires non-reciprocal motion. While not yet experimentally realized, we use molecular dynamics simulations to study the possible actuating states of circular magnetoelastic membranes and search for motion compatible with microswimming. We find precessing magnetic fields, above a critical frequency, can generate circumferentially and radially propagating waves, a type of non-reciprocal motion. We then introduce hydrodynamic effects using a lattice Boltzmann fluid. Truncating circular segments from the membranes allows for a circular swimming path and linear swimming can be achieved when the external magnetic field is programmed. The principles established here lay the foundation for the control and design of future magnetoelastic membrane systems.

**Chase** Brisbois received his B.S. in Nanoscale Science from SUNY Albany. He spent two years as a post-baccalaureate research fellow at the National Institutes of Health studying the structure of protein-lipid complexes called “nanodiscs”. His research work in the Olvera de la Cruz group at Northwestern focuses on the physics of magnetic composite materials using computational methods. Last year, he was a recipient of the International Institute of Nanotechnology's Outstanding Graduate Researcher Award. When Chase isn't furiously typing away on the computer, you may find him running along Lake Michigan or tending to the plants his cats have yet to destroy.

**Allessandra Dicorato**

B.A., Cornell University, 2015

## Multi-Scale Imaging of Nanomaterial-Tissue Interactions

Nanomaterials display extraordinary promise to revolutionize cancer treatment due to their biologically relevant size and tunable properties. Despite the abundance of therapeutics developed in the laboratory, however, as of 2019 only 28 nanomedicines were FDA approved. This lack of clinical translation is due, in part, to the array of barriers that may limit delivery of a therapeutic, which can make pinpointing a cause of failure challenging. To overcome this bottleneck, improved understanding of the nanomaterial/tissue interface is required, a task which demands visualization of nanomaterials in tissue at multiple length scales, from the micrometer length scales of subcellular compartments to the large scales of tumors themselves. In this work, we establish a multi-scale imaging platform that can be used to evaluate delivery of nanotherapeutics to cells and solid tumors. We demonstrate proof-of-concept by analyzing platinum-stabilized arsenic-loaded ‘nanobins’, as delivered to a patient derived xenograft model of glioblastoma. Using MRI, light microscopy, TEM, LA-ICP-MS, synchrotron XRF, cryogenic x-ray nanotomography, and XANES, we show that nanobins are delivered to the brain and tumor, are internalized within cells, and may enter cell nuclei. We further show that arsenic glutathione may be a major metabolite in cells. Finally, we illustrate that arsenic and platinum are transported differently in the cell through endosomal recycling, implying that arsenic, the drug’s cytotoxic agent, escapes the endosomal pathway, which can limit therapeutic delivery. Our platform is highly generalizable and may be extended to other systems, thus offering a systematic approach to expedite translation of nanomaterials to the clinic..

**Allessandra** DiCorato earned her BA in Chemistry and Chemical Biology with minors in Biomedical Engineering and English from Cornell University in 2015. As an undergrad, she worked in the biomineralization research group of Professor Lara Estroff, studying the bio-inspired growth of hybrid materials. She is currently a 6th year PhD candidate in Professor Derk Joester's group, where she uses multi-scale imaging techniques to study the interactions between nanomaterials and tissue that arise in two contexts -- in the development of calcitic endoskeletons in sea urchin embryos, and in the delivery of an arsenic-based therapeutic to glioblastoma tissue. She is a member of the Chemistry of Life Processes T32 Traineeship, Ryan Fellowship, and AAAS Mass Media Fellowship communities. In her free time, Allessandra enjoys reading, writing, baking birthday cakes for friends, and finding new neighborhoods and parks across the city.

## Ramya Gurunathan

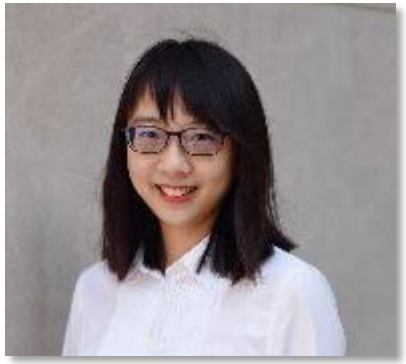
B.S. Materials Science and Engineering, Penn State University, 2016

M.Phil Scientific Computing, University of Cambridge, 2017

### Predicting the Thermal Resistance of Grain Boundaries and Interfaces

Heat management is an often a bottleneck for device efficiency, in technologies ranging from power electronics to thermoelectric modules. These same materials and devices tend to contain a high density of grain boundaries and interfaces, which, depending on the application, may need to be either thermally conductive or thermally resistive. As a result, models which can predict the thermal boundary (or Kapitza) resistance ($R_K$) from information about interface chemistry, structure, and type are highly impactful and can enable theory-guided thermal engineering of materials. However, the current standard theory for $R_K$ only considers the bulk properties of the material surrounding the interface and neglects the defect structure of the interface itself. Here, we develop a continuum-level model for $R_K$ which explicitly considers scattering due to the dislocation strain present at low-energy grain boundaries and interfaces. We apply this model to compare the thermal resistance of Si twist and tilt grain boundaries as well as the Si-Ge heterointerface. In addition to improving the accuracy of the predictions, the dislocation strain model reproduces trends observed experimentally and computationally between thermal resistance and grain boundary angle and energy. Finally, we can estimate the percentage contribution of dislocation strain scattering to the overall $R_K$, which may be tunable through annealing and control of microstructure, versus the acoustic mismatch scattering, which is typically fixed for a given material. In summary, we devise a simple, scalable model for thermal boundary resistance $R_K$, which retains important physical relationships between $R_K$ and interface structure.

**Ramya** is a PhD candidate in Prof. Jeff Snyder's group at the Northwestern Materials Science and Engineering Department. She received her B.S. in Materials Engineering at Penn State University. She then traveled to the University of Cambridge on a Churchill Scholarship and earned an MPhil in Scientific Computing. In her PhD, Ramya is working to model the interactions between heat-carrying phonons and structural defects. She has received the Cabell, Data Science Initiative, and PPG fellowships while at Northwestern. Outside of research, she currently serves as a graduate representative to the department diversity, equity, inclusion (DEI) committee and stays involved in science outreach through programs like Science Club. Ramya likes to make the most of the Chicago seasons with winter ice hockey and summer lake swimming.



## Chunyi Huang

B. Eng., Tsinghua University, 2016

### Doping control in nanowires for quantum computing

The manipulation of Majorana zero modes (MZMs) in semiconductor nanowire networks has been proposed as a means of quantum computing. The basic recipe is putting a superconductor in proximity to a semiconductor nanowire with strong spin-orbital coupling. The leading material candidates are InAs nanowires. In this work, we grow the branched InAs nanowires at a wafer scale with GaAs nanomembranes as templates by molecular beam epitaxy (MBE). However, it is very challenging to control the nanowire morphology and dopant incorporation simultaneously. With the help of atom probe tomography (APT), a time-of-flight technique that is capable of 3D compositional measurements at atomic scale, we have made progress towards self-assembled nanowires with the target doping profile, namely, remote doping. During the process, we have studied the nature of dopant incorporation and evolution of growth facets. This work lays the groundwork for doping control in scalable nanowire networks, including materials beyond InGaAs.

**Chunyi** is a fifth-year PhD student in Lauhon group. She received her Bachelor of Engineering degree at Tsinghua University (THU). While at THU, she did research on thermochemical cyclic splitting of CO2 catalyzed by metal oxides in Prof. Duan Weng's group. She also has some experience on soft materials when she worked on self-assembly of block copolymers in Prof. Alexandra-Katz group in MIT. At Northwestern, her research focuses on characterization of III-V heterostructures, more specifically, understanding the correlation between doping, strain and growth interface evolution. In her spare time, Chunyi enjoys traveling, WERQ, playing the piano and reading.

## Haiyue Huang

B.S., Shanghai Jiao Tong University, 2017

### On-mask Chemical Modulation of Respiratory Droplets

Mask wearing has become a new norm in many parts of the world in the COVID-19 pandemic. There has been much interest in enhanced masks that can better protect the wearers. However, a mask or face covering is much more effective in protecting others because it can block and reroute a large portion of the virus-laden respiratory droplets from symptomatic or asymptomatic infected wearers. Here, we propose an on-mask chemical modulation strategy to enhance this function by making the escaped droplets less infectious. As a proof of concept, antipathogen agents (e.g., mineral acid and copper salt) preloaded on nonwoven fabrics are shown to transfer to and are concentrated in escaped droplets to the level capable of deactivating pathogens. We hope that this approach leads to additional work, which, if eventually adopted, can help to cut down the sources of transmission and strengthen the public health response to control and mitigate the outbreak of infectious respiratory diseases.

**Haiyue** is a doctoral candidate in the Department of Materials Science and Engineering at Northwestern University, where she works with Prof. Jiaxing Huang on processing and assembly of two-dimensional materials. She is also developing healthcare materials and innovations for better and safer living.

## Nanoparticle Synthesis in Hollow Silica Shell Nanoreactors

Nanoparticle synthesis within nanoreactor templates has recently emerged as a highly attractive group of methods to synthesize complex nanoparticles. A nanoreactor template is simply an isolated volume with maximum feature lengths less than ~1 μm, which limits mass transfer of particle precursors and nanoparticles across the reactor periphery. Nanoreactors are attractive because reactor size and chemical contents can be used as modular handles to determine the final particle product, without excessive synthetic fine-tuning. This talk describes the strengths and challenges associated with hollow silica shell reactors and proposes a new strategy for addressing these challenges. Specifically, large individual nanoparticles within a template shell are taken as the desired particle product, as incomplete coarsening within a reactor typically results in particles of random or inconsistent stoichiometry. Herein, we describe a technique to improve the yield of desired particle products by studying how polymers can enhance gold nanoparticle coarsening within hollow silica shells.

**Liban Jibril**

B.S., Chemical Engineering, University of California, San Diego, 2017

**Liban** is a fourth-year Ph.D. candidate in Materials Science and Engineering, working with Professors Chad A. Mirkin and Vinayak P. Dravid. Prior to Norhwestern, he earned his B.S. in Chemical Engineering from the University of California, at San Diego. His current research focuses on unconventional approaches to control nanoparticle synthesis, specifically confined-template approaches, termed nanoreactors. He earned the Northwestern Ryan Fellowship from the International Institute for Nanotechnology, as well as the National Science Foundation Graduate Research Fellowship. In his free time, he enjoys watching T.V., playing sports, and suffering through Arsenal games.

**James Male**

B. S. Materials Engineering, Rensselaer Polytechnic Institute, 2017

## Improving doping in lead chalcogenide thermoelectrics

Defects are utilized in materials design to optimize properties of next generation devices like thermoelectrics, solid-state batteries, fuel cells, and photovoltaics. Semiconductors, in particular, must be doped for their many technological applications. However, the subtle effects of thermodynamics on defects and doping efficiency in semiconductors are often overlooked. Thermoelectric semiconductors perform best with degenerate carrier concentrations, meaning new materials might be held back by poor doping efficiency. Indeed, inconsistent performance is pervasive in the thermoelectrics literature, which harms the perceived reliability of thermoelectric devices. This study examines phase equilibrium and doping in n-type PbTe to provide a pedagogical framework for consistently synthesizing high-performance thermoelectric semiconductors. A saturation annealing technique is used to a explore the thermodynamic pathways leading to both the highest doping efficiencies and performance in PbTe. The best performance is found to be reproducible only when excess Pb is added to the structure through saturation annealing. Shortcomings in the literature are thus attributed to compensating vacancy defects caused by a simple deficit of Pb. The concepts applied here linking phase equilibrium to doping efficiency are understandable with a basic materials science education. Applying such concepts beyond lead chalcogenide thermoelectrics can ensure reproducible, optimal, and reliable performance in both new and classic materials systems.

**James** is a 4th year PhD student in the Department of Materials Science and Engineering, advised by Professor G. Jeffrey Snyder. He obtained his B.S. in materials engineering from Rensselaer Polytechnic Institute in 2017. James works closely with NASA's Jet Propulsion Laboratory as part of the NSTGRO fellowship to make thermoelectric materials more reliable using basic thermodynamics. Despite living in the flat Midwest, James is an avid snowboarder, camper, and hiker. In non-pandemic times, James loves traveling to conferences and going to concerts without worrying about strangers breathing on him.

**Kelly Parker**

B.S., Stanford University, 2016

## Soft Microscopy: Advancing High-Throughput Characterization at Low-Voltage

The structure-function relationship is essential to our understanding of materials systems; it spans length scales from atomic structure and chemical makeup to nano- and microscale properties and architecture to bulk or device-level function. Electron microscopy (EM) provides essential capabilities for the characterization of soft and biological structures, but the challenges associated with soft imaging are two-fold: Soft materials have low inherent contrast, and the electron dose required to achieve reasonable contrast causes significant damage. With rapid development of new materials and constructs, particularly in synthetic biology, imaging can be the bottleneck for complete characterization. While precedent often encourages cryo-EM when imaging biological structures, other methods can be higher-throughput and more easily accessible depending on the length scale of the sample and the resolution required to image essential features. Imaging at lower voltage than in typical transmission electron microscopy (TEM) is highly underutilized for biological materials, and it can significantly improve contrast. Many commercial scanning electron microscopes (SEMs) implement transmission detectors under the sample and allow for transmission imaging (STEM) at less than 30 keV. We have imaged protein assemblies using various STEM modes in an SEM at beam energies as low as 5 keV, and we can resolve individual proteins and their orientation in the complex. This technique offers both high-resolution and high-throughput structural characterization, is compatible with multimodal imaging and innovations for SEM, and can be extended to a range of soft and biological structures.

**Kelly** is a fifth-year PhD candidate in Professor Vinayak Dravid's group. She received her B.S. from Stanford University, where she researched silica degradation in cells for theranostic applications using electron microscopy. Her internship at the Leibniz Institute for New Materials in Saarbrücken, Germany solidified her interest in "seeing the invisible" through advanced characterization. Her work at Northwestern focuses on the development of microscopy methodologies to image biological structures, particularly through contrast enhancement in high-throughput imaging. Kelly is invested in improving diversity and inclusion in STEM fields through outreach and leadership, especially in her three-year role as GradSWE's Outreach Chair. She is also a flute player and classical music enthusiast, and she plays piccolo (the smaller flute) in Chicago's "Windy City Winds" community ensemble.

**Luke C. O. Prestowitz**

B. S., Nanoscale Engineering, University at Albany, State University of New York, 2015

## Towards Nanoarchitectonic Materials

Imagine that you are the architect assigned to build the great pyramid of Pharaoh Kufu—a royal tomb to put all others to shame. This task means you must build it for all to see, make it shine like a diamond under the desert sun, and ensure it lasts for millennia to establish the Pharaohs name.

Given this lofty goal, you must now select the materials necessary to assemble such an architectural feat. Starting with granite and limestone, you then need to fashion them into blocks of exact dimensions. The granite provides strength, the limestone a reflective surface. Stone slab by stone slab, held together by gypsum mortar, you start to build the pyramid. With time, it rises from the Sahara sands to tower above the horizon.

Although no Pharaoh has ordered such a great pyramid be built today, the process to develop nanoarchitectonic materials is different only in scale. The desired outcome—new and improved properties—is achieved by choosing the correct elemental building blocks, utilizing suitable syntheses to shape them, and constructing the final form through proper processing procedures. As a proof of this concept, we have chosen the silver nanowire as a model. The polyol synthesis assembles the silver atoms into a unique five-fold twinning structure, and through coating these blocks with copper “mortar”, we can assemble them to produce a bulk nanostructured metal. This material consists of a preserved proportion of the original nanowire structure, providing a basis for further development to build greater materials.

I am a 6th year student and a member of the Huang group. I went to SUNY at Albany for undergrad, which was a big help in preparing me for long interminable winters. My research is focused on developing processing frameworks to take nanoscale entities and, hopefully, turn them into useful materials. I enjoy the intersection of science, faith, and philosophy, and enjoy reading books or conversing with friends on said topics.

**Sonal Rangnekar**

B.S., UC Berkeley, 2016

# An Aerosol-Jet-Printed Graphene Biosensing Platform for Electrochemical Diagnostics

Sonal V. Rangnekar[1], Kshama Parate[2], Cicero C. Pola[2], Dapeng Jing[2], Deyny L. Mendivelso-Perez[2], Shaowei Ding[2], Ethan B. Secor[1], Emily A. Smith[2], Jesse M. Hostetter[2], Carmen L. Gomes[2], Jonathan C. Claussen[2], Mark C. Hersam[1]
[1]Northwestern University [2]Iowa State University

Inexpensive and rapid diagnostic biosensing is needed more than ever and may be achieved through the development of disposable electrochemical sensors. Graphene films are an ideal material for electrochemical biosensing due to their high electrical conductivity, large surface area, and biocompatibility. However, graphene films fabricated through chemical vapor deposition are too expensive for single-use applications, and low-cost manufacturing alternatives, such as screen and inkjet printing of graphene inks, do not provide sufficient control over electrode geometry to achieve favorable electrochemical sensor performance. In this work, aerosol jet printing is leveraged to pattern solution-processed graphene inks into high-resolution interdigitated electrodes (IDE) on a flexible polyimide substrate. After thermally curing in air, the IDEs are heated in $CO_2$ to create additional oxygen moieties on the graphene surface that are then reacted with EDC-NHS chemistry. The resultant graphene biosensing platform can be functionalized with arbitrary antibodies and blocking agents to create a highly sensitive and specific biosensor. This platform has been demonstrated for electrochemical detection of cytokines interleukin-10 and interferon-gamma to monitor immune system function (i.e., diagnosis of paratuberculosis in cattle) and for detection of histamine in food safety applications (i.e., determining fish spoilage). The high-resolution electrode geometry enables analyte sensing ranges and limits of detection that are appropriate for the respective applications. Furthermore, the biosensors are mechanically robust and withstand hundreds of bending cycles at high curvatures with minimal change in electrical and electrochemical signals. Overall, the low cost of manufacturing and short testing time (~30 min to soak and sense) motivate the expansion of this printed graphene biosensor platform into other sensing applications, including wearable health monitoring and human health diagnostics.

**Sonal** is a fifth-year PhD candidate in Professor Mark Hersam's research group. She earned a B.S. in chemical engineering & materials science and engineering at UC Berkeley. At Northwestern, Sonal's research focuses on the formulation of 2D material electronic inks for applications ranging from printed graphene COVID biosensors to black phosphorus IR cameras. Sonal is a 3M Graduate Fellow, HMCP Fellow, NU Center of Leadership Fellow, the current AVS Student Chapter President, and former Social Chair of GradSWE. Her drive to share scientific innovations with the world has motivated her to participate in the Medill science writing class and the Kellogg NUvention medical entrepreneurship program. Outside of the lab, Sonal is a semi-professional dancer and has led Bollywood dance classes for NU students.

**Travis Schmauss**

B.S. Materials Science and Engineering, Johns Hopkins University, 2016

## Surface Modification of Solid Oxide Electrodes for Robust Energy Storage

Fuel cells are electrochemical conversion devices that take a fuel and strip it of its electrons to generate electrical energy – oxidation, but without an open air “burn.” Solid oxide fuel cells (SOFCs) facilitate this process at elevated temperature (550°C-850°C) to avoid having to use expensive noble metal catalysts, as well as allowing the devices to oxidize more complex fuels than hydrogen, i.e., hydrocarbons and alcohols. This talk focuses on improving the functional lifetime of SOFCs through surface modification – as catalysts, much of the decomposition in their performance happens at the solid-gas interface. Understanding the processes that alter surface composition allow us to engineer better devices, staving off the most deleterious effects and even giving us insight into performing “resets” as maintenance of the SOFC stacks. The former will be investigated by means of atomic layer deposition (ALD), a method to deposit exactingly small amounts of materials into the high surface area electrodes; SOFC groups have had varying success with ALD, and this talk will explain the likely reason why. Later, the “resetting” mechanism will be shown to be possible with next generation fuel electrodes which only sprout their metallic active sites when exposed to fuel. By re-exposing them to air, the hands of time can be turned backwards on certain kinds of decomposition in order to generate fresh material -- to then be re-reduced in fuel. Together with carbon-based fuels, these are two ways of building the next generation of energy storage systems capable of massive energy transfer at scale.

Materials science has always been the most fascinating branch of science to me, and I've known this since long before I knew the name of the field. Originally from Southern California, I transplanted to the east coast for a degree at Johns Hopkins, cutting my research teeth working on reactive, multilayer thin films as an anti-weapon for anthrax defeat. I went from energetic materials to energy materials when I then transitioned to working with Prof. Scott Barnett here at Northwestern. I now study solid oxide fuel cells, both their initial and sustained performance, for their use in the green energy future -- at the grid-scale and vehicular level, both. I am the current president of the Northwestern Energy Technology Group and an ISEN Cluster Fellow.

**Donghoon Shin**

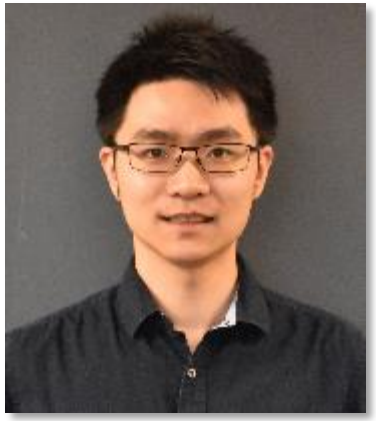
B.S., Hanyang University, South Korea, 2014,

M.S., Seoul National University, South Korea, 2016

## Bridging the Gap Between Halide Perovskite Nanocrystals and Thin-Films: Mesoscale Halide Perovskite Arrays

Halide perovskites have exceptional optoelectronic properties, but a poor understanding of the relationship between crystal dimensions, composition, and properties limits their practical use in integrated devices. Indeed, there is a lack of available synthetic approaches or subsequent perovskite research in the meso- regime between the nanoscale and the microscale, resulting in a property gap. Mesoscale perovskites may have properties that deviate significantly from those found in either regime. Herein, based on solvent evaporation synthesis, we report a new multiplexed cantilever-free scanning probe method for synthesizing compositionally diverse and size-controlled halide perovskite crystals. A polymer pen lithography (PPL), consisting of polydimethylsiloxane (PDMS) micro-pyramid pen array, delivers a small amount of precursor ink to the specific position, which leads to the mesoscale halide perovskite crystal arrays as the solvent gradually evaporates. In addition to the precise positioning of individual crystals, this method enables fine-tuning the crystal size by controlling ink concentrations and ink volume. This size tunability enables us to study optoelectronic properties as a function of crystal size systematically. This materials-versatile technique can be exploited to synthesize a wide range of perovskite materials and study their optoelectronic properties for a seamless regime without the study of property gap. Finally, the ability to sequentially pattern multi-color light-emitting single crystals in an array opens avenues towards more sophisticated optoelectronic devices, including a wide variety of optical displays.

**Donghoon** earned B.S. and M.S. in Materials Science and Engineering from Hanyang University, South Korea, in 2014 and from Seoul National University, South Korea, in 2016. Before joining Northwestern, he studied the ion-transport behaviors of oxide perovskite under thermal gradients. His current Ph. D. research focuses on halide perovskite nanocrystals and their array with polymer pen lithography method. He has received the 2020-2021 PPG Fellowship. In his free time, Donghoon spends time watching movies, enjoying art exhibitions.



**Raymond Wang**

B.S., Fudan University, China, 2016

## Learning the Crystal Structure Genome for Property Classification

Although numerous machine learning models have been developed to decode the structure-property relationship of crystalline materials, most of them explicitly include chemical composition in the feature set. Would it be possible to marginalize compositional information for generic solid-state materials and quantitatively study the correlation between crystal structure and materials properties? Here, we present a feasible solution to this question by utilizing a novel deep neural network (DNN) that learns directly from the momentum space structural genome to predict materials properties. Specifically, X-ray diffraction (XRD) patterns in the form of discrete 3-dimensional (3D) scattering points within momentum space are used as the only input features for the model to successfully accomplish multiple tasks: crystal system, elasticity, metallicity, and stability classifications. We design the neural network architecture to be robust against multiple invariance requirements inherent in the 3D XRD patterns. We find that different materials properties have various dependencies on crystal structures; we learn that crystal symmetry plays a significant role in determining the metallicity of a material, whereas electron density information contributes more to elastic properties. Materials stability prediction, on the other hand, is more chemical composition relevant; thus, our structure-based model is inferior to other DNNs that learn from compositional features. We also visualize the decision-making process of the metal-insulator classifier and identify some trends for materials with similar crystal structures. This work demonstrates the feasibility to use DNN models to help scientists understand materials physics (i.e., structure-property relationships) rather than only building predictive models. Our findings here also emphasize the significance of crystal structures to certain materials properties, which could potentially help decouple the structural and compositional optimization processes in functional materials design tasks.

**Raymond** is a Ph.D. candidate in Computational Chemistry. He obtained his B.S. degree at Fudan University, China. His Ph.D. research is mainly focused on data-driven materials design and discovery using machine learning and developing parallel computing algorithms for quantum molecular systems. Raymond specializes in high-performance computing, statistical learning, and parallel programming.

## A Hierarchically Structured Microparticle Platform for Regenerative Medicine

In the regeneration of complex tissues, such as the interface between cartilage and bone, there is a need to combine the tunability of synthetic biomimetic materials with spatial control of advanced manufacturing techniques. Bottom-up synthesis can be used to achieve precise structural control within scaffolds, but these methods are not always compatible with a wide range of biological environments. In this talk, I will discuss the development of a platform for creating microparticle-based inks from self-assembling peptide amphiphile nanofibers and how this can be used for constructing a hierarchy of structures within the tissue scaffolds. Specifically, utilizing a centrifugal microfluidic methodology, we show control over microparticle porosity and fiber superstructure utilizing a combined approach with biopolymer and peptide amphiphile interactions. This platform holds promise for the creation of well-defined cellular environments using techniques such as 3D printing.

**Kristen Wek**

BS/MS, Case Western Reserve University, 2017

**Kristen** is a fourth year PhD student in the Stupp group. Prior to studying at Northwestern University, Kristen completed her BS/MS in Macromolecular Science and Engineering at Case Western Reserve University. She is a recipient of the NSF Graduate Research Fellowship and her graduate research is focused on developing tunable tissue scaffolds utilizing 3D printing of extracellular matrix mimicking materials. Outside of the lab, Kristen has enjoyed baking and drawing throughout the pandemic and looks forward to snorkeling and hiking once she can travel.

*Thank you for attending!*

*Winners will be announced*

*at 5:00 PM CT.*

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