Northwestern ENGINEERING

Materials Science and Engineering

### 2023 John E. Hilliard Symposium

May 18, 2023

#### 8 AM to 4 PM

Ford Motor Company Engineering Design Center Evanston Campus ITW Auditorium, Room 1-350

**Keynote Speaker:** Kelsey Stoerzinger, Ph.D. Oregon State University

Cover art courtesy of Center for Hierarchical Materials Design (CHiMaD)

### **40th Annual Hilliard Symposium**



The John E. Hilliard Symposium is the Department of Materials Science and Engineering's annual capstone event, where we highlight the original research of our senior graduate students.

In its 40th year, this symposium encourages communication between our department and representatives of companies and agencies that support our work. It is also an opportunity to welcome back alumni, highlighting career paths and successes of our graduates.

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.

### **Keynote Speaker**

#### Kelsey Stoerzinger, Ph.D.



**Keynote Address:** "Working at the Interface: Navigating Junctions within Materials and Disciplines"

There are many times throughout our educational and career trajectories that we are asked to define ourselves and our science. These classifications can be helpful in developing a common language and toolset, but can at other times limit our insight and impact. I will share how my career and our lab's research in electrocatalysis has benefited from embracing intersectionality—such as between academic disciplines, classes of materials, scientific approaches, and institutions.

Kelsey Stoerzinger is an Assistant Professor in the School of Chemical, Biological and Environmental Engineering at Oregon State University. Her research group focuses on designing and understanding electrocatalysts that are selective and efficient in reactions for energy storage and chemical transformations. Stoerzinger holds a joint appointment at Pacific Northwest National Laboratory, where she was a Linus Pauling Distinguished Postdoctoral Fellow until 2018. She completed her doctoral studies in Materials Science and Engineering in 2016 from the Massachusetts Institute of Technology, supported by a Foundation Graduate Research National Science Fellowship. Stoerzinger received an M.Phil. in Physics from the University of Cambridge as a Churchill Scholar and a B.S. from Northwestern University. She is the recipient of awards including the MRS Nelson "Buck" Robinson Science and Technology Award for Renewable Energy, ISE Electrochemical Materials Science Award, Intel Rising Star Faculty Award, NSF CAREER, and DOE Early Career Awards.

# Schedule

8:00 AM	Breakfast & Registration - Ford ITW Auditorium		
8:50 AM	Welcome: Derk Joester - Ford ITW Auditorium		
9:00 AM	Presentations Begin - Ford ITW Auditorium		
9:00 AM	Roger Reinertsen — Bedzyk Group "Ion-Mediated Assembly of DNA-Functionalized Nanoparticles in Concentrated Electrolytes"		
9:15 AM	<b>Ruth Lee</b> — Stupp Group "Hierarchical Assembly of Peptide Amphiphiles Enhances BMP2 Delivery"		
9:30 AM	Michael Toriyama — Snyder Group "Topological Insulators for Thermoelectric Applications"		
9:45 AM	Lidia Kuo — Hersam Group "Sterilizable and Sustainable UV-Resistant Graphene– Polyurethane Elastomer Composites"		
	Break at 10:00 AM		
10:15 AM	<b>Christopher Hareland</b> – Voorhees Group "A CALPHAD Model of Non-equilibrium Dendritic Growth for the Additive Manufacturing of Industrial Alloys"		
10:30 AM	Anthony Silvaroli – Shull Group "Structure-Property Relationships and Design of Hybrid Silicone Elastomers"		
10:45 AM	<b>Kathleen Mullin</b> – Rondinelli Group "High-throughput Materials Discovery with Nanoparticle Megalibraries"		
11:00 AM	Keynote Address: Kelsey Stoerzinger "Working at the Interface: Navigating Junctions within Materials and Disciplines"		

# Schedule

12:00 PM	Lunch - Allen Center Speakers, Judges, Advisors: proceed to Allen Center (boxed lunches provided for attendees)	
1:15 PM	Hector Manuel Lopez de la Cerda Rios – Olvera Group "The Mechanics and Training of Nanoparticle Magnetoelastic Sheets"	
1:30 PM	<b>Carolin Wahl</b> – Dravid/Mirkin Group "High-throughput Materials Discovery with Nanoparticle Megalibraries"	
1:45 PM	<b>Carlos Torres</b> – Bedzyk Group "Material and Interface Engineering in Superconducting Quantum Circuits"	
	Break at 2:00 PM	
2:15 PM	<b>Simon Egner</b> – Stupp Group "Nucleic Acid Delivery Via Length-Controlled RNA-Binding Peptide Amphiphile Nanofibers"	
2:30 PM	<b>Lindsay Chaney</b> – Hersam Group "High-Temperature Microsupercapacitor Arrays Enabled by Printable Ionogel Electrolytes"	
2:45 PM	Jerren Grimes – Barnett Group "Enhancement of Ni-YSZ Fuel Electrode Performance Via Pressurization and GDC Infiltration"	
	Break at 3:00 PM	
3:15 PM	<b>Phil Staublin</b> – Voorhees Group "An Orientation-field Model for Grain Growth in Cubic Systems"	
3:30 PM	YuLing Chen – Shull Group "Deep Eutectic Solvents as Environmentally Friendly Solvents for Processing of Starch Polymers"	
3:45 PM	End of Symposium	

# Schedule at a Glance

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8:00 AM	Breakfast & Registration	Ford ITW Auditorium
8:50 AM	Welcome: Derk Joester & Peter Voorhees	Ford ITW Auditorium
9:00 AM	Student Speaker 1: Roger Reinertsen	Ford ITW Auditorium
9:15 AM	Student Speaker 2: Ruth Lee	Ford ITW Auditorium
9:30 AM	Student Speaker 3: Michael Toriyama	Ford ITW Auditorium
9:45 AM	Student Speaker 4: Lidia Kuo	Ford ITW Auditorium
10:00 AM	Break	Ford ITW Auditorium
10:15 AM	Student Speaker 5: Christopher Hareland	Ford ITW Auditorium
10:30 AM	Student Speaker 6: Anthony Silvaroli	Ford ITW Auditorium
10:45 AM	Student Speaker 7: Kathleen Mullin	Ford ITW Auditorium
11:00 AM	Keynote Address: Kelsey Stoerzinger	Ford ITW Auditorium
12:00 PM	<i>Lunch</i> Speakers proceed to Allen Center (boxed lunches provided for attendees)	Allen Center
1:15 PM	Student Speaker 8: Hector Manuel Lopez de la Cerda Rios	Ford ITW Auditorium
1:30 PM	Student Speaker 9: Carolin Wahl	Ford ITW Auditorium
1:45 PM	Student Speaker 10: Carlos Torres-Castanedo	Ford ITW Auditorium
2:00 PM	Break	Ford ITW Auditorium
2:15 PM	Student Speaker 11: Simon Egner	Ford ITW Auditorium
2:30 PM	Student Speaker 12: Lindsay Chaney	Ford ITW Auditorium
2:45 PM	Student Speaker 13: Jerren Grimes	Ford ITW Auditorium
3:00 PM	Break	Ford ITW Auditorium
3:15 PM	Student Speaker 14: Phil Staublin	Ford ITW Auditorium
3:30 PM	Student Speaker 15: YuLing Chen	Ford ITW Auditorium



Roger Reinertsen (he/him) Ph.D. Candidate, Northwestern University B.S., State University of New York

Ion-Mediated Assembly of DNA-Functionalized Nanoparticles in Concentrated Electrolytes

Many energy technologies require concentrated electrolytes to store and transmit energy. In spite of their utility, out understanding of the complex ion-ion and ionsolvent effects that govern the behavior of concentrated electrolytes is limited. This work utilizes interactions between highly charged DNA-functionalized gold nanoparticles to study electrostatic forces in concentrated salt solutions. Small-angle X -ray scattering measurements reveal that divalent cations induce the reversible crystallization of these nanoparticles into face-centered cubic, body-centered cubic, or amorphous structures. The type of structure formed depend on cation type and concentration. Interparticle separations within the assemblies exhibit a nonmonotonic dependence on salt concentration; the structures contract with added salt at low salinity, but swell when salt is added at high salinity, where classical theory predicts electrostatic forces to be of negligible range. Observations from wide-angle Xray scattering and molecular dynamics simulations implicate ion-ion interactions as driving this unexpected swelling at high salt concentration. Changing the solvent mixture to one with lower dielectric permittivity increases the electrostatic coupling in the system and enhances these effects. This work demonstrates continuous evolution of interactions between charged objects as salt concentration increases to saturation, providing insight on how ion-ion correlations shape how electrolytes interact with charged materials.

**Roger Reinertsen** is a Ph.D. candidate in Materials Science and Engineering working with Prof. Michael Bedzyk. Originally from Staten Island, New York, he decided to pursue the study of materials after a summer internship in zoo medicine convinced him that materials innovations were key to improving animal (and human) health. Pivoting from biology to semiconductors, he earned a B.S. in Nanoscale Science from the State University of New York at Albany in 2018, with his capstone research focused on characterizing transistor-based ion sensors. At Northwestern, his doctoral research focuses on using X-ray scattering to study colloidal assembly in concentrated electrolytes. His research has been supported by a Hierarchical Materials Cluster Fellowship and a PPG fellowship. Additionally, he has been honored with the prestigious "Most likely to be spotted drinking coffee" department paper plate award for four consecutive years. He cares deeply about science education, having served as a teaching assistant three times, and currently serves as an elected student representative on the Graduate Core Curriculum Committee. In his spare time, he enjoys drinking coffee, studying mixology, and developing games and quizzes.



Ruth Lee (she/hers) Ph.D. Candidate, Northwestern University B.S., Hope College

Hierarchical Assembly of Peptide Amphiphiles Enhances BMP2 Delivery

Peptide amphiphiles (PAs) are self-assembling molecules with great potential in regenerative medicine. BMP2-binding PA (BMP2b), a PA modified to bind to bone morphogenetic protein-2 (BMP2), has shown promise in applications for bone regeneration, particularly in spine fusion studies. Interestingly, BMP2b must be co-assembled with a diluent PA without the bioactive functional group to be efficacious. Herein, we link this requirement to differences in the structure of the supramolecular (co)-assemblies. We demonstrate that unlike the diluent PA that form well-dispersed fibers, and BMP2b that forms short fibers and micelles, co-assembly results in bundles of long nanofibers. Confocal microscopy and fluorescence-activated cell sorting (FACS) reveal that the co-assembled fiber bundles are internalized less rapidly, have higher BMP2 binding capacity, and slower BMP2 release. We conclude that bundling of fibers may prevent degradation and prolong the therapeutic effect of BMP2 for bone regeneration. This effect of a hierarchical assembly on the stability and kinetics of delivery is likely general and could aid in developing novel biomaterial platforms for protein delivery.

**Sieun Ruth Lee**, originally from Seoul, South Korea, is a 5th year PhD candidate in materials science and engineering. Under the mentorship of Prof. Samuel Stupp, Ruth's doctoral research focuses on studying peptide-based supramolecular polymers for applications in bone regeneration. For her research, she was awarded the Biotechnology Training Program Cluster Fellowship in 2020. Prior to Northwestern, she received a B.S. in Chemistry at Hope College in Holland, Michigan. Outside of the lab, Ruth participated in the Management for Scientists and Engineers certificate program at the Kellogg School of Management and was the president of the Materials Science Umbrella Society (MSUS) from 2022-2023. She also led various science outreach efforts for middle and high school girls through GradSWE and teaches Cambodian students English online to help empower them to pursue college education. In her free time, she enjoys baking, going to concerts, running, and traveling.



Michael Toriyama (he/him) Ph.D. Candidate, Northwestern University B.S., University of Illinois at Urbana-Champaign

Topological Insulators for Thermoelectric Applications

The rising demand for cooling, including refrigeration and air conditioning, poses significant environmental and economic challenges; air conditioning alone is responsible for almost 20% of electricity use in buildings globally. Distributed thermoelectric cooling offers a viable solution, thus making optimization techniques critical for pushing the boundaries of thermoelectric applications. A common method for improving the thermoelectric performance of a material is by increasing the valley degeneracy. We show that the valley degeneracy in a material can be enhanced through band inversion, leading to the natural conclusion that topological insulators are promising thermoelectrics. Using a combination of k.p perturbation theory and density functional theory calculations, we show that electronic bands must be sufficiently inverted for a topological insulator to possess high valley degeneracy. The band inversion strength can be engineered by modulating atomic orbital interactions, which can be done by e.g. alloying or strain engineering. By tuning the band inversion strength in a topological insulator, the valley degeneracy can be enhanced by a factor between 2 and 48, leading to significant improvements in the thermoelectric performance. The study offers a unique band engineering technique for thermoelectrics by capitalizing on the electronic structure topology of a material.

**Michael Toriyama** is a 4th year Ph.D. candidate in Materials Science and Engineering. With his advisor, Prof. G. Jeffrey Snyder, his research focuses on discovering and optimizing thermoelectric materials using computational tools and theoretical methods. He earned a B.S. in Materials Science and Engineering and B.S. in Applied Mathematics at the University of Illinois in Urbana-Champaign in 2019. He is a recipient of the Barry Goldwater Scholarship and the DOE Computational Science Graduate Fellowship. He was a co-organizer of the Virtual Conference on Thermoelectrics in 2021 and 2022.



**Lidia Kuo-Kim (she/hers)** Ph.D. Candidate, Northwestern University B.S., Rice University

Sterilizable and Sustainable UV-Resistant Graphene– Polyurethane Elastomer Composites

Shortages of personal protective equipment (PPE) at the start of the COVID-19 pandemic caused medical workers to reuse medical supplies such as N95 masks. While ultraviolet germicidal irradiation (UVGI) is commonly used for sterilization, UVGI can also damage the elastomeric components of N95 masks, preventing effective fit and thus weakening filtration efficacy. Although PPE shortage is no longer an acute issue, the development of sterilizable and reusable UV-resistant elastomers remains of high interest from a long-term sustainability and health perspective. In this work, graphene nanosheets, produced by scalable and sustainable exfoliation of graphite in ethanol using the polymer ethyl cellulose (EC), are utilized as UV-resistant additives in polyurethane (PU) elastomer composites. By increasing the graphene/EC loading up to 1 wt %, substantial UV protection is imparted by the graphene nanosheets, which strongly absorb UV light and hence suppress photoinduced degradation of the PU matrix. Further, graphene/EC provides mechanical reinforcement, such as increasing Young's modulus, elongation at break, and toughness, with negligible changes following UV exposure. These graphene/EC–PU composites remain mechanically robust over at least 150 sterilization cycles, enabling safe reuse following UVGI. Beyond N95 masks, these UVGI-compatible graphene/EC-PU composites have potential utility in other PPE applications to address the broader issue of single-use waste.

**Lidia Kuo** (unofficially Kuo-Kim) is a 5th year NSF Graduate Research Fellow and Harvey Fellow in Professor Mark Hersam's group, where her research focuses on two themes- 1) printed two-dimensional (2D) electronic materials and 2) functional 2D composites. Prior to starting graduate school, she received her BS in Materials Science and NanoEngineering from Rice University where she researched 2D materials for water treatment technologies with Professor Jun Lou. She hopes to use her background to develop sustainable and advanced functional fibers/textiles in her future research career. Beyond the lab, she is interested in teaching and educational outreach; her greatest hobbies are singing, playing bass guitar, and thrifting. You can find her on her secondhand 'fits blog, @sustainablepeasant on Instagram.



Christopher Hareland (he/him) Ph.D. Candidate, Northwestern University B.S., Rice University

A CALPHAD model of nonequilibrium dendritic growth for the additive manufacturing of industrial alloys

Additive manufacturing (AM) is of great interest in modern metallurgy, prompting the development of complex multicomponent alloys to optimize the properties of AM components. Due to the highly non-equilibrium processing conditions encountered during AM, this has led to a renewed interest in rapid solidification modeling. However, much of theory describing rapid solidification was developed for dilute binary alloys, limiting its usefulness to the AM of industrial alloys. Herein, we first derive a set of thermodynamically self-consistent interfacial response functions (IRFs) to determine the interfacial conditions (i.e., temperature and compositions) during rapid solidification of these alloys. These IRFs are then incorporated in a model of multicomponent dendrite growth, the dominant solidification morphology in metal alloys. This model is coupled with CALPHAD (CALculation of PHAse Diagrams) methodology, enabling the dendrite growth kinetics to be computed under AM processing conditions. Finally, the model is applied to 316L stainless steel—a ubiguitous industrial alloy used in applications ranging from nuclear reactors to biomedical implants to food processing-to address conflicting reports in the recent literature of its primary solidification microstructure during AM.

**Christopher Hareland** is a fourth-year Ph.D. candidate in Materials Science & Engineering working in the Voorhees group. His current research applies thermodynamics and kinetics to develop analytical models of non-equilibrium phase transformations (e.g., rapid solidification) in concentrated multicomponent alloys, which are coupled with CALPHAD methodology. Prior to Northwestern, he received a B.S. in Materials Science & NanoEngineering from Rice University in 2015, where he developed an ultrasonic powder compaction process (a variant of ultrasonic welding) to synthesize bulk nanostructured materials. Outside the lab, he enjoys playing tennis, reading, music, and photography.



Anthony J. Silvaroli (he/him) Ph.D. Candidate, Northwestern University B.AS., University of Waterloo

Structure-Property Relationships and Design of Hybrid Silicone Elastomers

Silicone elastomers demonstrate excellent surface, optical, and thermal properties that make them optimal materials for applications such as sealants, coatings, and high performance rubbers. However, these materials typically require mechanical reinforcement for applications requiring robust mechanical performance. Hybrid silicones made from interconnected polymer networks of PDMS and polymethacrylates can provide silicone-based elastomers with improved stiffness, toughness, and extensibility. In this talk, I explore the structure-property relationships that link composition and cure conditions to the resulting phase structure and mechanical performance of these hybrid materials. Using a Design of Experiments statistical approach, I investigate a wide range of material parameters, resulting in a vast array of materials with properties spanning several orders of magnitude. Based on the observed trends, a design strategy is crafted for these silicone-organic hybrids which allows them to be tailored for specific applications.

**Anthony Silvaroli** is a Ph.D. candidate in the Department of Materials Science and Engineering. He studies the mechanical properties and design of hybrid polymer materials under Professor Kenneth Shull. Anthony grew up in Mississauga, ON, just outside of Toronto. He obtained a Bachelor's of Applied Science degree in Nanotechnology Engineering from the University of Waterloo in Canada in 2018. Following his graduation, he will be working at Dow Chemical Company in Midland, MI as a Senior Research Specialist in Materials Science R&D. When he isn't doing research, Anthony enjoys cooking new meals, learning about history, and enjoying all sorts of sci-fi and fantasy entertainment.



Kathleen Mullin (she/her) Ph.D. Candidate, Northwestern University B.S., Illinois Institute of Technology

High-throughput Materials Discovery with Nanoparticle Megalibraries

The discovery of new materials is central to many aspects of society. Surveying the enormous parameter space for multi-component systems requires synthesis and screening platforms that are compatible with combinatorial high-throughput approaches. Nanoreactor lithography (NRL) has enabled, through the deposition of polymeric nanoreactors from scanning probe tips and subsequent thermal annealing, the preparation of megalibraries of up to 5 billion positionally encoded nanoparticles. However, its reliance on nanoparticle nucleation and growth in the nanoreactor has been an important constraint on chemical diversity. I will report on our recent expansion of NRL nanoparticle synthesis from 8 to 54 different metals, using a phase-separating nanoreactor design that enables nanoparticle formation through the direct sintering of a precursor aggregate. This expansion presents an unprecedented opportunity for the rapid mapping of complex phase spaces with the megalibrary platform. I will discuss our approach to addressing this challenge by developing fully autonomous, high-throughput workflows combining electron microscopy with artificial intelligence. For instance, we developed a braininspired framework of convolutional neural networks with physics-informed architectures to deduce the crystal systems of nanoparticles from arbitrarily oriented diffraction patterns. Taken together, our advances in high-throughput megalibrary synthesis and screening using autonomous electron microscopy may revolutionize materials discovery.

**Kathleen Mullin** earned her B.S in Materials Science and Engineering in 2018 from Illinois Institute of Technology in Chicago, IL. She is currently a PhD candidate in the Materials Theory and Design group lead by Professor James Rondinelli. Her research centers on using computational models to understand the materials physics of molecular qubits for quantum sensing applications. Outside of research, she served as the treasurer for the Materials Science Student Association from 2019-202. She enjoys reading, baking, and playing tabletop games.



Hector Manuel Lopez de la Cerda Rios (he/him) Ph.D. Candidate, Northwestern University

The mechanics and training of nanoparticle magnetoelastic sheets

In computational devices memory is encoded by the flipping of dipoles in response to a magnetic field. In materials science, a close but insufficient analogue are stimulus-responsive materials that can change their properties in response to environmental conditions. However, they often offer limited tunability during manufacturing and cannot be reconfigured on the fly. Trainable materials break this paradigm in that they can be taught to which degree to alter their properties in response to environmental changes. To be able to "learn", materials must have reconfigurable internal degrees of freedom, and they must be able to retain these newly reconfigured states. Here, we study the mechanics of magnetoelastic sheets, of hvdrocarbon-coated superparamagnetic nanoparticles composed that are manipulated with magnetic fields. Our collaborators have shown repeated deflection and heating cause the membrane to retain more and more deflection each cycle, thereby training the membrane into new configurations. Our molecular dynamics simulations suggest that this training results from the hydrocarbons coating the particles reconfiguring in the deflected state when heated. Due to the combined insights of simulation and experiments, magnetic nanoparticle sheets are an ideal platform for the exploration of general principles of mechanical training of materials.

**Hector Manuel Lopez de la Cerda Rios** is a fifth year graduate student in Materials Science and Engineering at Northwestern University, studying in the group of Monica Olvera de la Cruz. He is interested in active matter due to its macroscopic dimensions and reconfigurability as a function of external fields within timescales of only seconds to minutes. These materials have the potential to adapt to their external environment thus eliciting life-like behavior in inanimate matter, which may accelerate the advancement of autonomous machines (similar to what cybernetics was intended to accomplish). When he is not working on his academic projects, he likes to go to the Green Mill to listen to jazz, analyze cultural divides, ponder about science and that which we cannot comprehend (largely inspired by science fiction by Stanislaw Lem), watch all kinds of movies, and play the harmonica.



**Carolin Wahl (she/hers)** Ph.D. Candidate, Northwestern University M.S., Northwestern University B.S., University of California, Santa Cruz

High-throughput Materials Discovery with Nanoparticle Megalibraries

The discovery of new materials is central to the advancement of society as it has direct impact on the practical application of materials such as polymers, batteries, catalysts, and many others. Nanomaterials in particular have unusual properties that primarily arise due to their spatial dimensions (<100 nm). To adequately survey the enormous parameter space for nanomaterials design, synthesis and screening platforms that are compatible with combinatorial high-throughput approaches are required. Having developed a generalized lithography method for nanoparticle synthesis that allows for the incorporation of up to 54 different metals into nanoparticles enables combinatorial materials synthesis, the subsequent screening of the resulting megalibraries is particularly challenging on the nanoscale, where the necessary high-fidelity characterization tools are limited in their ability to perform high-throughput measurements. To that end, we are developing an electron microscope-based screening platform for libraries of nanoparticles. This approach provides compositional and crystallographic information to determine the structures of these largely unknown materials. Working with up to 108 nanoparticles per library necessitates transforming the way we traditionally use electron microscopes, both in terms of instrument time for data acquisition and the operator's time for data analysis. Autonomous workflows such as this result in challenges associated with data processing, which must contend with massive volumes of data and be performed in real time to provide feedback to the running instrument. At this scale, the incorporation of artificial intelligence becomes critical at numerous points during the process, with algorithms continuously drawing conclusions from the data to make informed decisions about how to proceed. In building platforms like this, there is an immense opportunity to expand the scope of using electron microscopes: beyond the manual study of individual materials and towards autonomous systems for high-throughput characterization.

**Carolin Wahl** is a Ph.D. candidate in Materials Science and Engineering at Northwestern University. She studied both Chemistry and Computer Science at the University of California, Santa Cruz and received her Master's degree in Materials Science and Engineering from Northwestern University. Working with Profs. Chad Mirkin and Vinayak Dravid, she develops methods for rapid synthesis of nanomaterial libraries and integrates them with Al-enhanced high-throughput structural and functional screening platforms to accelerate the discovery of new materials. She is also involved in the commercialization of these discovery technologies across industries.



**Carlos G. Torres-Castanedo (he/him)** Ph.D., Northwestern University M.S., CINVESTAV, Mexico

Material and interface engineering in superconducting quantum circuits

Quantum computers hold great promise for computational tasks where conventional computers fall short. From handling large datasets to solving molecular-level systems, quantum computing will have a substantial impact shortly. Superconducting qubits are among the most mature quantum platforms for multiqubit quantum processors. These devices are fabricated on commercially available silicon or sapphire wafers using well-known nanofabrication processes. Still, the challenge resides in building a nearly perfect device from many defective materials. Decoherence, the lifetime of a qubit, depends on the purity and nature of the materials employed. In this talk, the efforts to understand and mitigate mechanisms that lead to decoherence are presented. This in-depth exploration is possible with the use of a variety of non-destructive X-ray techniques. The correlation between materials and interfacial processing to superconducting device performance is presented.

**Carlos Torres** is a 5th-year Ph.D. candidate in Materials Science and Engineering, co -advised by Michael Bedzyk and Mark Hersam. He is originally from Mexico. Previously, he was a visiting student at Michigan State University in the USA and a visiting researcher at KAUST in Saudi Arabia. He was awarded the Fulbright Fellowship for his Ph.D. at Northwestern University, where he studies the electrode/solid electrolyte interface for Li-ion batteries using X-rays. As part of the Superconducting Quantum Materials and Systems Center (SQMS) collaboration, he is further interested in connecting interfacial and bulk properties of superconducting thin films with decoherence mechanisms. His work involves X-ray characterization, thin film deposition, and surface processing. He wishes to continue his academic career as a postdoc and faculty. Outside the lab, he loves to travel and learn from different cultures. He enjoys experimenting with exotic cuisines and passionately follows his favorite soccer team.



Simon A. Egner (he/him) Ph.D. Candidate, Northwestern University B.S., University of Illinois at Urbana-Champaign

Nucleic Acid Delivery Via Length-Controlled RNA-Binding Peptide Amphiphile Nanofibers

Messenger RNA therapies can reprogram the body's healing processes by directing cells to produce specific proteins, including those not naturally produced by the target tissue. However, RNA instability remains a major obstacle, and current RNA therapies, such as vaccines, are delivered systemically with little cellular uptake specificity. Localizing RNA to specific tissues using protective, bioactive nanostructures offers the possibility to treat diseases through multiple pathways with minimal off-target effects. Here, a poly(ethylene glycol)-functionalized peptide amphiphile molecule capable of binding nucleic acids and self-assembling into colloidally stable nanofibers was developed. By design, the RNA binds to the interior of the nanofiber. Protecting it from degradation in this way may enable fabrication of a locally injectable biomaterial that mimics the extracellular matrix and has regenerative properties. The RNA binding PA demonstrated a micelle-to-fiber transition with significant thermal hysteresis, enabling the seeded growth of monodisperse, length-controlled nanofibers. Control over the nanofiber length can be used to modulate cell uptake. There is great potential in using the described nanofiber delivery of mRNA for the treatment of debilitating conditions like chronic spinal cord injury.

**Simon A. Egner** earned a BS in Materials Science and Engineering from the University of Illinois at Urbana-Champaign in 2019. He is now a fourth year Materials Science and Engineering PhD student in Professor Samuel I. Stupp's group at Northwestern University. His research focuses on understanding the kinetics and thermodynamics of peptide supramolecular polymerization, particularly in multi-component systems. Outside of research, Simon serves as a graduate fellow in Northwestern's Brady Scholars Program, an academic program centered on ethics and civic duty. He also enjoys playing intramural sports and board games.



Lindsey Chaney (she/her) Ph.D. Candidate, Northwestern University B.S., University of California, Los Angeles

High-Temperature Microsupercapacitor Arrays Enabled by Printable Ionogel Electrolytes

Rising demand for portable electronics and sensing networks for the Internet of Things continues to drive innovations in the energy storage sector. In order for these devices to run remotely, they must be able to self-sufficiently store their own energy and thus require compact, integrated power sources. Microsupercapacitors are an excellent option due to their exceptionally long cycle lives and their rapid energy delivery and uptake. Additionally, their planar device architecture is easily integrated with all components of a wireless device, allowing for streamlined manufacturing directly on a single substrate. In this work, we demonstrate fully screen-printed, flexible microsupercapacitor arrays via rapid deposition of a hightemperature hexagonal boron nitride (hBN) ionogel electrolyte. The hBN ionogel can be printed onto large-area ( $\sim 100 \text{ cm}^2$ ), graphene-based microsupercapacitor arrays within seconds, enabling mass-manufacturing. The devices have an areal capacitance of 0.9 mF cm<sup>-2</sup>, which rivals the best graphene-based devices to date. In addition, unlike incumbent polymer-based electrolytes, hBN ionogel electrolytes exhibit stable cycling at high temperatures up to 180°C. Elevated operating temperatures result in an increase in power density and enables self-powered, remote devices to be deployed in harsh, high-temperature environments such as underground exploration, aviation, and electric vehicles. This combination of highperformance functionality in harsh conditions and a scalable fabrication strategy significantly expands the application space for microsupercapacitors.

Lindsay Chaney is a PhD candidate in the Hersam Lab at Northwestern University. She received her B.S. from UCLA in Chemistry/Materials Science in 2015 and then began working at the UCLA-based spinoff SuperMetalix to help commercialize academic work on superhard borides. In 2018, she began her PhD at Northwestern, where her work focuses on large-scale synthesis of graphene nanoplatelets and the development of functional inks for printed electronics. She is an NSF Graduate Research Fellow and enjoys mentoring high school students weekly at the Chicago Boys & Girls Club. Outside the lab, she enjoys rock climbing, cycling, and playing with her cat Cheeks.



Jerren Grimes (he/him) Ph.D. Candidate, Northwestern University B.S., Tufts University

Enhancement of Ni-YSZ Fuel Electrode Performance Via Pressurization and GDC Infiltration

With the transition to renewable energy resources like solar and wind well underway, working around their intermittency will be an increasingly important consideration. Electrochemical grid storage solutions address this problem by offering efficient storage during times of excess energy production and rapid transition to energy supply when demand increases. For example, reversible solid oxide cells (ReSOCs) create fuel from excess electricity in electrolysis mode and electricity from stored fuel.

Before widespread adoption, ReSOCs must satisfy three fundamental conditions: (i) high performance, (ii) long operational lifetime and (iii) low overall cost. Pressurized operation typically results in a lower area-specific resistance, which translates to improved round-trip efficiency and can offset performance losses due to lower temperatures typical for long-lasting devices. Modifying the electrode surface via the infiltration of gadolinium doped ceria nanoparticle catalysts has recently been shown to offer additional performance improvements. However, there is little literature data that explores pressurized ReSOC operation. Furthermore, the effect of pressure on the catalytic activity of ceria nanoparticles in this context is largely unknown.

Herein, we investigate the effects of temperature, pressure, infiltration, and water humidification level on the polarization resistance associated with the most common fuel electrode material: Nickel – Yttria Stabilized Zirconia (Ni-YSZ). A symmetric cell setup is used to isolate the response from air electrodes that would be present in a full cell. Electrochemical impedance spectroscopy (EIS) is used to determine polarization resistances and equivalent circuit modeling using a custom Python script is used to better understand the different processes occurring within the cell under different conditions. These results are used to inform a general model that can be used for predicting future full cell performance under similar conditions.

Jerren Grimes is a 5th year PhD Candidate in the Barnett Research Group in the Materials Science and Engineering department. His research investigates electrochemical systems for energy production and storage with a focus on the reversible solid oxide cell and electrode development. Here, he has explored methods for characterizing degradation mechanisms, extending their operational lifetime, and improving their performance. Prior to his work at Northwestern University, he was a research engineer at Lockheed Martin Advanced Energy Storage working on their novel redox flow battery technology in Cambridge, MA. Following graduation, he hopes to obtain an R&D role within the renewable energy space with a continued focus on electrochemistry. Outside of research, he enjoys cooking, swing dancing and trying his hand at various photography styles.



Phil Staublin (he/him)

Ph.D. Candidate, Northwestern UniversityM.S., Michigan Technological UniversityB.S., Michigan Technological University

An Orientation-field Model for Grain Growth in Cubic Systems

Properties of metal materials, such as conductivity, corrosion resistance, and mechanical strength, depend strongly on the grain boundaries present in the material; therefore, predictive models of grain growth are critical to controlling materials properties in processes such as additive manufacturing. Grain boundaries are characterized by five macroscopic crystallographic degrees of freedom: the misorientation between the adjoining crystals and the inclination of the boundary plane. Because the grain boundary energy and mobility can depend on these degrees of freedom, models for grain growth must incorporate the boundary crystallography while respecting the underlying crystal symmetry. Current models which incorporate all five degrees of freedom are often expensive to compute or fail to reproduce analytical theories of boundary motion. We present an orientation -field model for grain growth in which the grain boundary energy and mobility depend on all five macroscopic degrees of freedom. The model uses a single-well potential and incorporates crystal symmetry using an expansion in symmetrized hyperspherical harmonics, and because only one order parameter is needed, this model is more memory efficient than commonly used multi-phase-field methods. We demonstrate the model's ability to reproduce equilibrium trijunction dihedral angles and equilibrium crystal shapes for cubic anisotropy. Simulations of polycrystals show a pronounced effect of low angle grain boundaries when these boundaries are assigned lower energies, demonstrating the importance of varying grain boundary energy on the microstructural evolution. With the ability to include both arbitrary crystal symmetry and crystallographic dependence of grain boundary properties, this model shows promise for simulating grain growth phenomena in a wide range of material systems.

**Phil Staublin** is a PhD candidate in the Voorhees research group. He earned his B.S. in Materials Science and Engineering from Michigan Technological University, where he also later received an M.S. degree in Materials Science. His M.S. thesis research studied precipitation kinetics in dilute aluminum-zirconium alloys. At Northwestern, he studies grain growth in polycrystalline metals, developing novel phase-field modeling techniques which incorporate the many degrees of freedom in grain boundary evolution. He was Treasurer for the Materials Science Student Association at Northwestern for 2019-2020. In his free time, Phil enjoys rock climbing, cooking, and playing board games.



YuLing Chen (she/hers) Ph.D. Candidate, Northwestern University

Deep Eutectic Solvents as Environmentally Friendly Solvents for Processing of Starch Polymers

Low-Density Polyethylene (LDPE) is a popular plastic material that is widely used due to its low cost, flexibility, and ease of processing. However, the long lifespan of LDPE and its contribution to plastic pollution have increased the demand for more sustainable alternatives. One promising alternative is thermoplastic starch (TPS), which is derived from natural and renewable sources such as corn, potatoes, and cassava. TPS shares similar properties with LDPE, such as flexibility and processability, but is biodegradable and compostable, making it a more environmentally friendly option.

Despite its potential as a replacement for LDPE, TPS has faced several challenges in real-world applications. One of the main issues is the short shelf life caused by retrogradation, which occurs when the plasticizer evaporates, leading to a change in crystallinity within the film. Previous studies have shown that ionic liquids (ILs) can suppress retrogradation; however, the high cost of ILs has hindered their use in practical applications.

To address this issue, this presentation introduces deep eutectic solvents (DESs) as a sustainable alternative to ILs. This study explores the effectiveness of four different DESs as plasticizers for TPS in suppressing retrogradation. The research investigates the potential benefits of using DESs, including their ability to improve the stability and properties of starch polymers. Overall, this study highlights the potential of DESs as a sustainable and cost-effective solution for processing TPS to replace the LDPE in various applications, including packaging, agriculture, and consumer goods.

**YuLing Chen** is a passionate researcher with a strong focus on improving the polymer processing industry. Her current research is centered around finding innovative ways to improve the current processing methods, including utilizing deep eutectic solvents to enhance and stabilize polymer properties. Through her doctoral projects, YuLing has established a deep knowledge of innovative techniques that enhance the quality and efficiency of polymer processing. In her free time, YuLing enjoys baking, cooking, eating, and exercising, and is dedicated to maintaining a healthy work-life balance.

## **Campus Map**



### **MSE Department Vision Statement**

The Department of Materials Science and Engineering at Northwestern understands that true excellence requires diversity in a myriad of ways.

We affirm the profound value of diversity of thought as it arises from diversity of background, experience, race, ethnicity, gender/gender identity, sexual orientation, socioeconomic status, belief system, nationality, age, ability/disability, veteran status, and marital and family status. We are committed to proactive outreach to recruit, support, and promote those from underrepresented and underserved populations. Inclusion, equity, and engagement are essential to the well-being of our diverse community. We acknowledge our responsibility to foster equitable educational and professional outcomes across our department, and to ensure that all members are safe from harassment arising from differences. Thus, we actively strive to create an environment that is anti-racist, anti-sexist, and anti-biased in all ways, while celebrating the differences that enrich our intellectual and personal discourse. Integral to our pursuit of academic excellence and rigor is a supportive environment of mutual respect in which we engage in open, inclusive discussion and vigorous debate. This is how great ideas are born and nourished.

We invite you to join us, hand in hand, with partners from all walks of life, on our mission to expand the frontier of knowledge.

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