Greetings from the Department of Chemical Engineering and Materials Science (ChEMS) at Michigan State University! The past few years with the pandemic have been challenging. Nevertheless ChEMS has been very busy and has had several productive years. Here are some of the exciting highlights and achievements of our students, faculty, and staff.

**NEWS**

- **Donald Morelli**, Professor of Materials Science, who has led the ChEMS Department with keen professionalism and skill as chair or interim chair for the past six years, stepped down from the chair position August 2021. He has been an outstanding leader who has worked on behalf of everyone in the department. I was appointed Interim Chairperson of ChEMS on August 16, 2021.

- MSU alumnus **Bill Hargreaves** has generously recognized Professor **Martin Hawley**’s contributions to the department, university, and profession by funding the Martin C. Hawley Endowed Chair in honor of Martin Hawley. We are deeply grateful for Bill’s tangible recognition to the extraordinary commitment Marty has made to ChEMS and MSU. His legacy will continue through future faculty members who will hold the Martin C. Hawley Endowed Chair, and who will reflect the leadership and commitment to MSU that Martin Hawley has set throughout his career.

- Professor **Martin Hawley** elected to retire in May 2022. Professor Hawley has served MSU in multiple administrative roles, including as co-director of the NSF Center for Low-Cost High-Speed Polymer Composites Processing from 1991 to 2001, as chairperson of Chemical Engineering and Materials Science (ChEMS) from 2001 to 2015 and, since 2015, as director of the Composite Vehicles Research Center and senior associate dean of the College of Engineering. While chairperson of ChEMS, the faculty size in the department increased by about 50%, the student body nearly doubled, and research expenditures for the department increased by a factor of five.

- Due to the diligent efforts of **Anne Eisenlohr** and **Maddalena Fanelli** and several MSE faculty members the move of several MSE courses and a ChE course to the new STEM Teaching and Learning facility was seamless and a success. This new STEM building facilitates interdisciplinary connections within STEM and across disciplines, and provides experiential learning opportunities for students in STEM.

**NEW FACULTY**

With programs in both chemical engineering and materials science and engineering, research in ChEMS spans a remarkably wide range of topics, including the metallurgy of lightweight alloys, materials for energy storage and conversion, polymers and composites for structural and functional applications, new materials and nanotechnology, bio-based and biorenewable products, and biomedicine. This expertise and range of interests have been further enhanced in the past three years as we have welcomed six new faculty members to the department, and another joining in 2023:

- **Caroline Szczepanski**, joined us as an Assistant Professor in Fall 2019. Dr. Szczepanski’s group develops techniques using polymers and polymer networks to produce materials for biomaterials, coatings, plastics, membranes, and adhesives.

- **David Hickey**, joined us as an Assistant Professor in Fall 2019. Dr. Hickey’s research focuses on the design of electroactive small molecules, molecular electronics, and polymer materials for a variety of applications related to energy storage, catalysis, and biosensing.

- **Daniel Woldring**, joined us as an Assistant Professor in Fall 2019. Dr. Woldring’s group develops high performance therapeutics and diagnostics using novel protein engineering methods.

- **Jose Mendoza**, joined us as an Assistant Professor in Fall 2020. Dr. Mendoza’s research focuses on the development and application of numerical techniques to study structural, electronic, transport and optical properties of materials, low-dimensional systems and nanostructures.

- **Chengcheng Fang**, joined us an Assistant Professor in Fall 2020. Dr. Fang’s group develops multiscale quantitative characterization tools, and designs advanced materials and manufacturing methods for energy storage and conversion devices.

- **Assaf Gilad**, joined the ChEMS faculty as a Professor in Spring 2022. He joined Michigan State University in the BME department in 2017. Dr. Gilad works to develop novel genetically encoded and nanoparticles biosensors for both brain imaging and neuromodulation.

- **Xinyue Liu**, a postdoctoral fellow at MIT, will join the ChEMS faculty in Fall 2023. Dr. Liu is developing soft material systems for environmental sustainability.

**PARTNERSHIPS**

In addition to research activities in ChEMS, our faculty are further strengthening and enhancing collaborative activities on campus and across the globe. New collaborations are being developed between ChEMS faculty and researchers at the Fraunhofer Center for Diamond and Coating Technologies, and several of our graduate students are involved in research in the Fraunhofer facility in the Engineering Research part of campus; a cohort of our faculty working in the biomedical arena continue to interface and collaborate with scientists in the Institute for Quantitative Health Science, and Engineering; and the dual-PhD degree programs with the Institute of Chemical Technology, Mumbai, the Indian Institute of Technology, Madras have brought students from these institutions to MSU for research.

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from the Chair
FACULTY AWARDS & HONORS

Our faculty members continue to excel in their work, and their success in doing so is reflected in the numerous prestigious awards and honors they have received this past year. Some highlights include:

- Donald Morelli received the 2021 Outstanding Achievement Award from the International Thermoelectric Society (ITS);
- Alexandra Zevalkink was the recipient of the 2021 NSF CAREER Award and the 2022 Withrow Distinguished Junior Scholar Award;
- Johansen Crosby Endowed Professor of ChEMS Richard Lunt received the 2022 MSU Tech Transfer Achievement Award;
- Chengcheng Fang was named one of the 35 Innovators under 35 by MIT technology review for 2022;
- Caroline Szczepanski and Carl Boehlert received Strategic Partnership Grants in 2022 from the Canadian Studies Center to develop joint research at Université Laval;
- Robert Ofoli was named the College of Engineering Faculty Excellence Advocate in 2021 and was the recipient of the 2022 Sustained Excellence in Diversity recognition;
- Carl Lira was the recipient of the 2022 Withrow Teaching Excellence Award
- Martin Crimp was the recipient of the 2022 Exceptional Service Award from the College of Engineering;
- Nichole Shriner received the title of Master Distiller on DiscoveryPlus and the winner of the Discovery Channel competition Moonshiners show in 2022;
- Assaf Gilad received the 2022 MTRAC Innovation Challenge Award.

STUDENT ACHIEVEMENTS

Students, of course, are the lifeblood of the academic enterprise, and once again this year several of them at both the undergraduate and graduate levels have received accolades for their outstanding work, including:

- Jenna Magness, ChE senior, won the 5000m and 10,000m Championships at the 2022 Big Ten Outdoor Track & Field at the University of Minnesota and was named the Women’s Track Big Ten Outdoor Athlete of the Championships in Minneapolis. Jenna placed 3rd in the Women's 10,000m - NCAA D1 Outdoor Championships and earned CoSIDA Academic All-America Third Team Honors.
- Bonnie Stolt (MSE undergrad), Emma Smith (CHE undergrad), Leah Schlesinger (CHE undergrad), and Shay Ladd (CHE undergrad) received College of Engineering Student Service Awards
- Evan Litch took first place in the 2021 AIChE Student Design Competition’s individual category; Austin Alexander took first place in the 2021 AIChE Student Design Competition’s Best Applications of the Principles of Chemical Process Safety Award in the Individual Category as well as second place in the 2021 AIChE Student Design Competition’s individual category. Austin Jenner and Ian Scheper won the Best Applications of the Principles of Chemical Process Safety in the 2021 AIChE Student Design Competition’s team category.
- ChE graduates Emma Smith, Ethan James, Carson Malhado, and Austin Kamer and MSE graduate Kevin Dunne received the Board of Trustees’ Award, MSU’s most prestigious academic honor
- MSE junior and alumni distinguished scholar Bonnie Stolt won 1st place in her category at the University Undergraduate Research & Arts Forum
- ChE doctoral student Kevin Chen received a best poster award in the Health and Biomedical category at the 2022 Engineering Graduate Research Symposium
- Apoorva Kulkarni, a PhD student has won the 2021-2022 outstanding graduate student award in Chemical Engineering and was also awarded the Extrusion Division Lew Erwin Scholarship from the Society of Plastic Engineers Foundation
- MSE junior Emma Ainsworth has been awarded a $1,500 scholarship from ASM International – Detroit chapter, the world’s largest association of materials-centric engineers and scientists
- ChE junior James VanAntwerp was nominated for a Goldwater Scholarship

DISTINGUISHED ALUMNI

Finally, our alumni continue to make us proud of our programs and their graduates. A few highlights for this year include:

- In May 2022, ChEMS BS alumnus John (Jack) Wilkens, CEO of Woundchek Laboratories, was awarded the 2022 Red Cedar Circle Distinguished Alumni Award. Woundchek is the first in class point-of-care diagnostics test for non-healing wounds.
- ChEMS Alumi Gary Hockstra and Karl J. Puttlitz were the Red Cedar Circle Award recipient in 2021 and 2020, respectively!

While we leave the last few years behind, the doors of tomorrow beckon us toward the future, and we are excited about the possibilities and opportunities that we will encounter. I hope you will enjoy reading the research highlights contained in this brochure, and I look forward to updating you on our progress in the future.

Christina Chan
University Distinguished Professor and Interim Chairperson
Department Highlights

The Michigan State University Department of Chemical Engineering and Materials Science (ChEMS) has vibrant research programs in both chemical engineering and materials science and engineering.

- **OUTSTANDING FACULTY**

  Among our 35 faculty members, we have:
  - Five NSF CAREER Award winners
  - Four University Distinguished Professors
  - Five MSU Distinguished Faculty/William J. Beal Outstanding Faculty winners
  - Six MSU Teacher-Scholar Award winners
  - Four Withrow Distinguished Scholar Award winners
  - Three Withrow Junior Scholar Awards winners
  - Ten Withrow Teaching Excellence Award winners (several have won multiple times)
  - Excellence in Diversity Award winner

  Also included among the faculty ranks are multiple society Fellows:
  - National Academy of Inventors
  - American Institute of Chemical Engineers (AIChE)
  - American Institute of Chemists
  - American Institute for Medical and Biological Engineering (AIBME)
  - American Society for Engineering Education (ASEE)
  - Society of Plastics Engineers (SPE)
  - ASTM International
  - American Ceramic Society
  - ASM International
  - ABET
  - American Physical Society (ASP)
  - The Minerals, Metals & Materials Society (TMS)
Many faculty members have also received national and international recognition for their academic and research achievements.

**DEPARTMENT ACHIEVEMENTS**
- Total research expenditures were over $7 million last year
- Approximately 125 refereed publications and 3 patents per year
- Total undergraduate student population to 490 (as of Spring 2022)
- Graduate enrollments of 79 PhD and 10 MS (as of Spring 2022)

**RESEARCH CENTERS**
The department operates a number of major research centers, including:
- The Composite Materials and Structures Center
- Institute for Advanced Composites Manufacturing Innovation (IACMI) Scale-up Research Facility (SuRF)

**PARTNERSHIPS**
In today’s world, partnerships with industry and global institutions play an ever-increasing role in research and innovation, and our department has been active in seeking and developing these connections.
- The Institute for Advanced Composites Manufacturing Innovation (IACMI) Scale-up Research Facility (SuRF) is and includes a host of industry partners working closely with ChEMS faculty and on lightweight polymer composites for vehicles at the prototyping facility in the Corktown area of Detroit.
- ChEMS and Dow are working to grow research collaboration and educational program on machine-learning, data-mining, and process optimization to further broaden the experiences of our students and help prepare them for tomorrow’s world
- ChEMS faculty and Fraunhofer researchers are building new collaborations to work with both federal agencies and industrial companies. These interactions will facilitate the sharing of expertise and equipment and resources.

**MISSION & GOALS**
The Department of Chemical Engineering and Materials Science pursues a mission of growing national recognition as a center of excellence in research, teaching, and service. In support of this mission the department has four goals:
- Leadership and excellence in conducting nationally recognized, innovative, and cutting-edge research
- Recruiting high-performing students and delivering modern, high-quality graduate and undergraduate programs that produce top-notch graduates serving the needs of industry, government, and academia
- Outstanding professional and outreach services
- Cultivating support from the private sector, state, and federal sources, and providing stewardship in support of research, instruction, and service.

**STRATEGIC INITIATIVES**
As we look to the future, the department has established strategic initiatives to ensure our continued ascension in productivity and prominence:
- Continued faculty growth to complement and supplement our research priorities
- Recruitment of a growing pool of high-quality PhD students
- Increased recruitment of highly qualified undergraduate students, and matriculation of bachelor’s degree graduates that are prepared to solve the problems of both today and tomorrow
- Enhanced support of endowments for fellowships, scholarships, professorships, and the discretionary excellence fund.
RESEARCH INTERESTS
Grain boundaries, crystallographic texture, crystal plasticity, microstructure evolution, damage nucleation

LAB(S)/GROUP(S)
Solder Research Group, Niobium Research Group, Titanium Research Group

WEBSITE
http://www.egr.msu.edu/~bieler/

SPECIAL EQUIPMENT AVAILABLE
Orientation imaging microscopy, in situ deformation stage in SEM

GROUP MEMBERS
Jiawei Lu and Zack Thune

PATENTS

CURRENT RESEARCH
Orientation imaging microscopy™ (OIM, aka EBSP mapping) is used to quantitatively examine the relationships between microstructure and localized deformation processes that ultimately control heterogeneous deformation, recovery and recrystallization mechanisms, and damage nucleation. Combined with other experimental and analytical tools, such as 3D x-ray diffraction, new insights on formability and damage nucleation mechanisms are found. This will enable development of optimal material processing strategies to gain more predictable and reliable properties. Four examples follow:

DAMAGE NUCLEATION IN TITANIUM AND TITANIUM ALLOYS.
Figure 1 shows a set of measurements of the local stress state in 1 μm voxels of commercial purity titanium in a 4-point bent sample under load. Differential Aperture X-Ray Microscopy allows the local deviatoric stress tensor at each voxel and the local crystal orientation to be measured. The stress is illustrated with ‘stress jacks’, which show the direction and magnitude (color) of the average stress in each grain (large jacks) and how the local state of stress varies significantly along grain boundaries and along the surface. Additional analysis of orientation gradients reveals local dislocation density that allows details of the slip deformation processes to be identified.

DOE/BES SISGR Grant, with M.A. Crimp, C.J. Boehlert, and P. Eisenlohr

MICROSTRUCTURAL IMPACT ON THE MACHINABILITY OF TITANIUM ALLOYS.
Machining of titanium is often the most expensive part of the process to make titanium parts, due to excessive tool wear. This grant will reveal underlying mechanisms that cause tool wear, and how tool-work piece interactions affect the properties of the machined surface. Relationships between microstructural evolution in the titanium work piece, the chip, and wear of the tool will be quantified. Recent results prove that the high tool wear rates with high speed machining are correlate with high temperatures that cause transformation to a softer (beta) phase that attacks the tool more severely.
NSF CMMI MEP, with P. Kwon (ME)

Microstructural evolution during thermo-mechanical cycling in lead-free solder joints. A set of solder joints were given incremental sets of thermomechanical cycling to determine how the damage process evolved. The long dwell times between increments of thermal cycling and X-ray measurements led to less than half of the number of cycles to failure than continuous thermal cycling until failure. This indicates that damage develops when not being cycled (used). In-situ High Energy X-Ray Diffraction (HE-XRD) identifies how the stress and crystal orientation evolved, and post-mortem sectioning of joints showed complimentary agreement between X-ray and Electron Backscattered Diffraction measurements (the EBSD measurement is on a plane, while the X-ray samples the entire volume of the joint).
(With Jason Quan Zhou.)
**Characterization and modeling of deformation of defects in high-purity Nb for particle accelerators.** High-purity Nb is used for radio frequency superconducting particle accelerator cavities (the structures that accelerate particles), but the fundamental physics of deformation and surface modification processes (which includes strong acid etching) and microstructure evolution are not well understood. Figure 3 illustrates how preferential magnetic flux penetration (red arrow) occurs along low angle grain boundaries, and may result from hydride precipitates that form during cooling. Hydrides leave scars when they dissolve upon reheating to room temperature. The hydride scars are misoriented by as much as 10° from the surrounding material, indicating that significant local straining occurred.

DOE/OHEP, with P. Eisenlohr and N.T. Wright (MSU), F. Pourboghrat (OSU), K. Solanki (ASU), and C. Compton (FRIB).

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**Recent Publications**


The search for absorbable metal systems, showing the occurrence of DRX during HPT.

Experimental set up of the HPT processing conducted in the Zn-Mg samples, (a) cross-sections of the Zn-Mg HPT-processed disks after 1, 5, 15, and 30 turns.
X-ray diffraction along with transmission electron microscopy (TEM) demonstrated that HPT was able to induce the nucleation of the intermetallic compounds, Mg$_2$Zn$_{11}$ and MgZn$_2$, identified close to the disk edges after 15 and 30 turns, see Figure 2. The volume fraction of these intermetallics increased consistently with the number of turns, as determined from Rietveld refinement. Similarly, an exceptional increase of the hardness values was recorded with increasing number of turns, with values over 250 HV after 30 turns at the disk periphery. These values are among the highest hardness values ever reported for the Zn-Mg alloy system, and it is due to the contribution of several strengthening mechanisms: Hall-Petch effect and hard intermetallic compounds.

Overall, these results have demonstrated that HPT exhibits potential for the development of Zn-Mg hybrid systems (at RT) with ultrafine-grained metal-matrix structures having enhanced hardness that may open a window towards the research of a new generation of medical device applications.

**Figure 2.** EBSD orientation maps, misorientation angle plots, basal (0001) pole figure of the Zn matrix near the periphery of Zn-Mg HPT disks after (a) 1 turn, (b) 5 turns, (c) 15 turns and (d) 30 turns. Imax is the maximum intensity observed in the pole figures.

**Figure 3.** (A) X-ray diffraction patterns taken from the mid-thickness plane at the periphery of the Zn-Mg HPT disks, (b) Bright-field TEM image and (c) corresponding selected area diffraction pattern from the periphery of the Zn-Mg HPT disk after 30 turns. The phases associated to the diffraction rings and their reflection planes are labeled in yellow.

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**RECENT PUBLICATIONS**


**RESEARCH INTERESTS**
Electrochemistry and electrocatalysis, from theory to experiment

**LAB**
Electrochemical Energy Lab (Engineering Bldg., 428 S. Shaw Lane, Room 3250)

**WEBSITE**
www.msu.edu/~scb

**GROUP MEMBERS**
STUDENTS & COLLABORATING FACULTY: James Woodworth (PhD), Carolina Carbray, Brandon Howard, Nick Quebbeman, Christina Wark, Yan Xie, and Yunlu Zhang

**PATENT**

**CURRENT RESEARCH**
Our research addresses engineering and materials issues in fuel cells, particularly mass transport within high-rate catalytic electrodes. We focus on non-precious metal catalysts based on redox enzymes and transition metals, which have low cost but often introduce transport limitations. We study these issues using experimental and multi-scale modeling approaches. Below are brief descriptions of current projects.

*Bio-inspired design of adaptive catalysis cascades.* As new catalytic systems are created for the production of advanced materials, energy conversion and harvesting, and human/machine interfaces, it is clear that natural pathways provide essential clues that will inspire novel designs. In this collaboration we are developing integrated catalytic cascades created from different catalytic modalities to optimize selectivity, electron transfer, diffusion, and overall pathway flux. The contribution of our laboratory is to quantitatively model the coupling of these novel catalytic steps and to study the transport of intermediates between steps (Figure 1).

We are currently studying the ability of electrostatic channeling to enhance cascade throughput and efficiency. We use multiscale simulations combined with advanced sampling techniques to understand the channeling mechanism, quantify cascade kinetics and design future cascades. Figure 2 shows an example of a cascade structure, synthesized by our collaborators, containing two enzymes joined by a positively-charged polypeptide. The negatively charged intermediate (G6P

2−
) is guided by electrostatic forces from one enzyme to the next. Molecular dynamic (MD) simulations demonstrate a hopping mechanism on the cascade surface, and we quantify energy barriers for hopping and desorption using techniques such as umbrella sampling and Markov State modeling. We are able to show clear ionic strength dependence of long-range and short range interactions. We are currently developing experimental capability to monitor intermediate distributions experimentally, using scanning electrochemical microscopy.

We have extended this approach to channeling by molecular confinement, exemplified by reactions within a carbon nanotube (CNT, Figure 3). Using continuum and molecular modeling techniques, we have demonstrated the geometric and transport parameters that will allow high retention and reaction of intermediates inside the CNT.

Sponsor: U.S. Army; Collaborators: Universities of Utah and New Mexico, Columbia University, University of California Riverside

*Metal nitrogen carbon (MNC) oxygen reduction catalysts for automotive fuel cells.* We are developing a new process for inexpensive Metal-Nitrogen-Carbon (MNC) catalysts for oxygen reduction cathodes. High-pressure pyrolysis yields active MNC catalysts from transition metal (iron or cobalt) and nitrogen precursors (pyridine, melamine) combined with high surface area carbon materials in a closed, constant...
volume reactor (Figure 4). Activity approaches that of precious-metal platinum in acid and alkaline electrolytes. We study the performance of these catalysts within a fuel cell cathode layer using numerical modeling techniques. Using our model, we have identified opportunities to optimize the design for improved performance, including reduced catalyst layer thickness and increased hydrophobicity of catalyst layer materials (Figure 5).

**Electrocatalytic hydrogenation using low-cost metal catalysts.** The advent of low-cost electricity creates an opportunity to convert biomass to value added fuels and chemicals by electrochemical hydrogenation at low temperatures and pressures. Furfural, for example, can be converted to furfural alcohol and methyl furan by hydrogenation, with applications in perfumes, polymers and pharmaceuticals (Figure 5). We are developing high surface area and low cost metal supported carbon catalysts for these reactions, wherein Ni, Cu, Fe are supported on activated carbon in molecular and nanoparticle form and their performance is screened on the basis of conversion and selectivity towards the desired products. Successful catalysts will enable new pathways for chemical products from renewable sources.

**Collaborator:** Inst. Chemical Technology, India
Christina Chan
University Distinguished Professor and Interim Chairperson
krischan@egr.msu.edu | 517-432-4530 | 428 S. Shaw Lane, Room 1243

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**RESEARCH INTERESTS**
Disease mechanisms, system biology, drug delivery, tissue engineering

**WEBSITES**
https://www.egr.msu.edu/people/profile/krischan
http://www.egr.msu.edu/changroup/

**LABS**
Cellular & Molecular Laboratory, Integrative Systems and Computational Biology Laboratory

**GROUP MEMBERS**
Joydeep Rakshit and Ryan Thompson
Co-advised with S. Patrick Walton: Kevin Chen and Chauncey Splichal
Undergraduate students: Sean Foster, Ryan Jin, Shay Ladd, and Caleb Sandum

**PATENT**

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**CURRENT RESEARCH**

**Biophysical mechanisms of palmitate-induced signaling and cytotoxicity.** Numerous diseases, including non-alcoholic fatty liver disease, cardiovascular disease, type 2 diabetes, metabolic syndrome, neurodegenerative diseases, and cancer, involve malfunction of the endoplasmic reticulum (ER) stress response. Physiological conditions such as elevated levels of saturated long chain-FFAs, e.g. palmitate, have been shown to induce ER stress in many types of cells, and to contribute to the development of these ER stress-associated diseases. We found that palmitate promotes the dimerization of inositol-requiring enzyme (IRE1α), an ER stress sensor protein, through the Trp457 residue in the transmembrane domain of IRE1α (Figure 1). This study will impact the design of therapeutics that target the ER stress response in treating metabolic dysfunction, as well as the design and development of drug therapies that target ER stress-associated diseases, including cancers, Alzheimer's disease and many other diseases.

**Delivery of siRNAs by polymeric nanoparticle**
(Collaborator: S. Patrick Walton). The overall goal of the proposed research is to design vehicles with optimal chemical and physical characteristics. The interactions of siRNAs with delivery vehicles built from chemically-diverse oligomeric and polymeric nanoparticles are quantitatively analyzed to determine those structural features that encourage complex formation and release of siRNAs into the cell.

**Neural transdifferentiation of MSCs through down-regulation of the NRSF.** Mesenchymal stem cells (MSCs) are multipotent adult stem cells exhibiting a high proliferation rate and plasticity as compared to other adult stem cell lines. MSCs naturally serve as precursors for adipocytes, chondrocytes, and osteocytes, and provide trophic support for cells of the immune system in the bone marrow. In vitro experiments have shown that MSCs can be induced to gain characteristics of neural cells including generation of Na⁺K⁺ currents, expression of neural specific structural proteins, and exhibition of neuronal morphology upon induction. Previously, we demonstrated that the cAMP-elevating agents, forskolin and IBMX, induced neural-like differentiation of MSCs, including expression of neural markers and increased sensitivity to neurotransmitters. However, due to the broad range of effects that forskolin and IBMX can elicit through the intracellular second messenger, cAMP, a better mechanistic understanding is required. Recently, we show that neural induction by forskolin and IBMX is dependent on downregulation of expression of the master transcriptional regulator, neuron restrictive silencer factor (NRSF), and its downstream target genes. Since silencing of NRSF is known to initiate neural
Differentiation, we found that forskolin and IBMX result in transdifferentiation of MSCs into a neural lineage (Figure 2).

**CRISPR to increase the homogeneity and efficiency of stem cell differentiation.** CRISPR to increase the homogeneity and efficiency of stem cell differentiation. Stem cells are a promising cell source for the regeneration of aged, injured and diseased tissues and organs, but to realize their therapeutic potential challenges remain, including restricting the growth of unwanted cell types and improving the efficiency of converting them to a specific cell type, and thereby render them safer to use. The heterogeneous nature of stem cells presents challenges in inducing them into a specific cell type. Early transplantation studies to treat Parkinson’s Disease successfully regenerated lost dopamine-producing neurons but also resulted in involuntary movements caused by the expression of other types of neurons. Therefore, reducing unwanted cell lineages by genome editing several genes through multiplexing via CRISPR would greatly enhance the efficiency of stem cell differentiation to a specific cell type, decrease probability of mutagenesis and render its use safer. Thus, the overall aim of the project is to increase the efficiency and specificity of stem cell differentiation by reducing off-target cell types through CRISPR. CRISPR/Cas9 mediated knockout of transcription factors involved in the maturation of serotonergic, glutamatergic and GABAergic phenotypes will be performed. We show that MSCs exhibit heterogeneous differentiation during dopaminergic differentiation. We aim to create Tbr1−/− MSCs that could potentially yield a more homogeneous dopaminergic population after induction with forskolin and IBMX.

**Figure 2.**

- 1. NRSF Neural Gene Repression
- 2. Induction with cAMP-elevating small molecules or NRSF silencing
- 3. Neural Gene Derepression
- 4. Gain of neural characteristics
- TuJ1+ -Neurotransmitter sensitivity

## Recent Publications

Shiwang Cheng
Assistant Professor
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- **RESEARCH INTERESTS**
  Dynamics of polymers at interfaces and its relationship to their rheological properties, polymer nanocomposites (including bio-based polymers) design, glass transition and glassy dynamics

- **WEBSITE**
  https://www.egr.msu.edu/people/profile/chengsh9

- **LABS**
  Dynamics and Mechanics of Soft Materials Group (Engineering Bldg., 428 S. Shaw Lane, Room 3535)

- **SPECIAL EQUIPMENT AVAILABLE**
  Broadband dielectric spectroscopy, Anton Paar MCR 302, Fabry-Pérot interferometer, Rheo-optics, Rheo-dielectrics

- **GROUP MEMBERS**
  GRADUATE STUDENTS: Matthew Melton and Shalin Patil
  COLLABORATORS: Dr. Yangyang Wang (ORNL).

- **PATENT**

**FIGURE 1.** Left: A sketch of chain conformations (microstructures) of polymer nanocomposite with low molecular weight. Short trains, loops, and tails can be expected in this case. Right: A sketch of chain conformations (microstructures) of polymer nanocomposite with high molecular weight. Large loops, long tails, and possible bridges can be anticipated in this case. The red and blue beads represent segments of adsorbed polymers. The olive beads represent segments of non-adsorbed polymers.

**FIGURE 2.** Rheo-dielectrics to probe the dynamics of interfacial polymers under active deformation. Special attention will be paid to the two types of events here: (i) forced polymer-nanoparticle detachment, (ii) force disentanglement between adsorbed polymers and their adjacent chains.

- **CURRENT RESEARCH**
  Polymers are promising candidates to address emerging challenges in environment, food, and energy. Understanding the structure-property relationships of polymeric materials are crucial to design novel polymeric materials on demand. The Dynamics and Mechanics of Soft Materials group are interested in the dynamics of multicomponent polymeric materials at different times and lengths scale, and their correlation to the microscopic properties. Currently, we are pursuing the structure-property relationship of multi-component polymeric materials from dynamics and mechanics perspective of view.

**Dynamics and mechanics of polymers at interfaces.** Polymers adsorbing onto a surface can form a variety of different microstructure such as trains, loops, and tails. Structurally, the population of each microstructure at the interfacial region varies with the polymer molecular weights, the polymer-nanoparticle interactions, and so forth. The complicated surface conditions have strong impacts on the structure and dynamics of interfacial polymers. For example, the polymer adsorption is typically known as an irreversible process with extremely long lifetime. So far, there are no experimental methods that enable one to effectively study the dynamics of polymers at the interface, especially the slow modes like the Rouse, sub-Rouse, and diffusion of interfacial polymers. In this project, we focus on the polymer structure and dynamics at the polymer/nanoparticle interface. With a combination of dielectric spectroscopy and rheology, we aim to understand the correlation between the properties of the interfacial layer of a few nanometers and the macroscopic properties of polymer nanocomposite, i.e., the mechanism of nano-reinforcement.

**Advanced polymer nanocomposites design.** Recently, we have demonstrated that small nanoparticles are much more effective in tuning macroscopic properties of PNCs than conventional big nanoparticles, suggesting a potential paradigm shift in PNCs design (Fig. 3). The advanced macroscopic properties of small nanoparticle PNCs (s-PNCs) include a large shift in glass temperature (~10× larger than conventional nanoparticle PNCs (c-PNCs)), an unexpectedly high fragility index (up to 270), a high threshold of kinetic gelation (> 40 vol%), an apparent “fully disentanglement” of polymers with molecular weight of 100 kg/mol, and a processing favorable zero-shear viscosity. We proposed the origin of the large effects as (i) a finite desorption time between the small nanoparticle and polymer segment; (ii) the high mobility of the nanoparticles; (iii) the small sizes. This discovery opens new routes of tuning the
establishment of a molecular deformation mechanism of glassy polymers. In this project, we plan to apply in situ rheo-spectroscopy measurements during mechanical tests to characterize the changes of the local vibrations (the “free volume”), the elastic heterogeneity length scale, and the activated segmental hopping during deformation. These details are all critical to illustrate the nature of the high mechanical stress, the origin of the shear yielding and toughening, and the molecular mechanism of the fracture of polymer glasses.

**RECENT PUBLICATIONS**


Martin Crimp
Professor
crimp@egr.msu.edu | 517.285.8321 | 428 S. Shaw Lane, Room 3513

- **RESEARCH INTERESTS**
  Deformation and fracture mechanisms, substructure characterization, nanoindentation, grain boundary strain transfer, electron diffraction and channeling, dislocation mapping, scanning electron microscopy, transmission electron microscopy

- **LABS**
  Electron Microscopy and Characterization (Engineering Bldg., 428 S. Shaw Lane, Rooms 3507 and 1130), Sample Preparation Facilities (Engineering Bldg., 428 S. Shaw Lane, Room 3510)

- **WEBSITE**
  http://www.chems.msu.edu/people/profile/crimp

- **SPECIAL EQUIPMENT AVAILABLE**
  Two field emission scanning electron microscopes with electron backscattered diffraction (EBSD) orientation mapping capabilities, including one dual column focused ion beam (FIB)/FEG-SEM; tensile, bending, and high cycle fatigue in situ deformation stages; heating and cooling stages

- **GROUP MEMBERS**
  PhD STUDENTS: Hailey Becker

- **CURRENT RESEARCH**
  The overall focus of this group is to develop and apply advanced electron beam characterization techniques. The group works on a range of interdisciplinary projects that deal with diffraction based imaging approaches, based on both scanning electron microscopy (SEM) and transmission electron microscopy (TEM). While the core research programs in this group deal with advancing the understanding of deformation and fracture in structural metals, collaborative studies have included magnetic multilayer structures, carbon nanotubes, ceramic joining, oxygen sensors, and cholesterol.

  **Characterization of deformation structures using scanning electron microscopy.** Enhancing the performance of metals and alloys used in structural applications requires an understanding of the mechanisms that lead to strength, toughness, and in particular, damage nucleation that leads to failure. For many years these mechanisms have been characterized using TEM, but this approach is limited by the need to use very thin samples with small fields of views. Here at MSU we have been at the forefront in the development of SEM approaches that allow the direct imaging and crystallographic characterization of deformation structures in the near surface regions of bulk samples using electron channeling contrast imaging (ECCI) (Figure 1). Recently, we have worked on extending this approach to 3-dimensional analysis of structure using serial imaging/tomography approaches based on both electropolishing and focused ion beam sectioning.

  **Characterization of heterogeneous deformation in polycrystalline arrays using ECCI.** The reliability of engineering structures is often limited by the development of local damage during processing or service. Such damage can often be traced back to the heterogeneous deformation that is inherent in polycrystalline metals. Thus, in order to optimize the performance of structural materials, it is critical to characterize the nature of deformation in these polycrystals, particularly at grain boundaries. We have recently developed a new ECCI-based approach for such characterization that allows identification of grain boundary dislocation nucleation sites as well as the manner in which dislocation slip bands interact with grain boundaries (Figure 2). Using this approach, we are identifying how different polycrystalline arrays may be more or less susceptible to damage nucleation, with an aim towards identifying optimum microstructures for structural applications. Recent 3D ECCI results have demonstrated how mis-aligned slip systems at grain boundaries can effectively transfer shear by nucleating small numbers of dislocations on a variety of planes, often with high critical resolved shear stresses (Figure 3). These small packets of dislocations then merge with the dominant slip bands to carry shear through the interiors of the grains.

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**FIGURE 1.** ECCI image of the dislocations produced during the propagation of a crack in NiAl.
Dislocation interactions at grain boundaries. Grain boundary engineered materials display enhanced strength and ductility over other polycrystalline materials. Many of these engineered microstructures contain large numbers of crystallographic twins. Understanding how dislocation slip interacts with the resulting twin boundaries is critical to further development of these materials. Working with Professor Yue Qi, we have been combining experimental observations of the dislocation interactions with twin boundaries with molecular dynamics atomistic simulations of the same processes (Figure 4). Matching the simulations with the nature of the experimentally observed dislocation pile-up allowed the barrier stress associated with the boundary to be determined.

RECENT PUBLICATIONS


RESEARCH INTERESTS
Energy, wealth, and human well-being. Integration of bioenergy generated using sustainable agricultural practices with electricity from solar and wind.

FACULTY COLLABORATORS
Dr. Seungdo Kim, Professor Wei Liao, Professor Chris Saffron

PATENTS

FIGURE 1. “Win-Win Outcomes from Biogasdoneright™“
CURRENT RESEARCH

Current global trajectories for food and energy production are not sustainable. There are currently over seven billion people on the planet and another two billion are expected in the next few decades. Therefore, food production must expand significantly and soon. But current food production practices tend to deplete soil and degrade water supplies. Modern agriculture uses large quantities of fossil energy both directly and indirectly and is thereby a major greenhouse gas emitter. Modern agriculture also depends heavily on synthetic pesticides and herbicides with many resulting adverse environmental effects.

Lack of energy access is at the root of human poverty. To provide energy services that will lift people from poverty we must also rapidly expand energy production. But about 85% of current energy use is based on fossil energy. If we expand energy production based on fossil energy resources, we will accelerate buildup of atmospheric greenhouse gases at the very time when we should instead be removing large quantities of carbon from the atmosphere and sequestering it in stable forms.

Agriculture is an industry, and like other industries, agriculture must be financially healthy if it is to innovate and become more sustainable. But prices of crop commodities are at historically low levels and many farmers are going bankrupt. How will agriculture innovate and become more sustainable if it does not have the required cash flow? Large scale, sustainable bioenergy production might provide the additional income.

However, we will not solve linked problems by addressing them in isolation. We must address linked problems as an integrated whole, using “win-win” approaches.

These unsustainable, strongly linked trends in food and energy production must be addressed now. We do not have decades to wait for “perfect” solutions. We need proven, scalable, sustainable approaches now. We can improve and innovate on these approaches as we proceed, but it is time to implement large scale, sustainable, “no-regrets” approaches to integrated food and energy production.

I am currently contributing to two efforts to sustainably integrate food and energy production. One is using the ammonia fiber expansion (AFEX™) process to produce high quality ruminant animal feeds from low quality straws and hay. AFEX-treated straws can also be used as feedstocks for producing biofuels such as ethanol. With support from the Gates Foundation, the AFEX process is now being scaled up to produce dairy animal feeds in India. The additional milk production enabled by the AFEX treatment will provide enough income to potentially lift millions of poor Indian families from poverty.

The second approach to integrated food and energy production is called Biogasdoneright™, or BDR. BDR is a set of linked practices for sustainable on-farm production of food linked with both production and conservation of energy. BDR depends on double-cropping to produce energy crops for anaerobic digestion. These energy crops represent additional carbon extracted from the global carbon cycle. Energy crops, plus crop residues, manures and agrowastes, are converted to biogas, electricity or biomethane. Stable carbon and plant nutrients are recycled to the soil through the residual digestate stream to reduce farmer costs and sequester carbon in the soil. The BDR approach with its many linked “win-win” outcomes is summarized in Figure 1.

Bioenergy systems modeling is supported by the Department of Energy, Great Lakes Bioenergy Research Center.

RECENT PUBLICATIONS


B.E. Dale, “Feeding a sustainable chemical industry: Do we have the bioproducts cart before the feedstocks horse?,” Faraday Discussions (2017).

Lawrence Drzal
University Distinguished Professor
drzal@egr.msu.edu | 517.353.5466 | 428 S. Shaw Lane, Room 2100

- **RESEARCH INTERESTS**
  Polymer-fiber composite materials, nano-composites (graphene, halloysite, silica), bio-composites (bast fibers, cellulose nano-fibrils, cellulose nano-whiskers), fiber-polymer interfaces (carbon, glass, uhmwpe, aramid), adhesion, adhesive bonding, nanostructured electrodes for batteries and supercapacitors

- **LAB**
  Composite Materials and Structures Center

- **WEBSITES**
  http://www.chems.msu.edu/people/profile/drzal
  www.egr.msu.edu/cmsc

- **SPECIAL EQUIPMENT AVAILABLE**
  Specific instrumentation available for the fabrication, evaluation, characterization and testing of polymer, fibers, nanoparticles and their polymer composite materials:
  - **COMPOSITE MATERIALS EVALUATION AND ANALYSIS**
  - **COMPOSITE MATERIALS FABRICATION**

- **GROUP MEMBERS**
  PHD STUDENT: Christopher Cugini

- **SELECTED PATENTS (37 TOTAL)**

- **CURRENT RESEARCH**
  - **Nanostructuring of multifunctional graphene nanoplatelet composites for structural, energy generation and energy storage applications.** The Drzal research group is in general conducting research in polymer composites including: polymer composites reinforced with fibers and nanoparticles (graphene and cellulose), processing of composites, adhesion, biobased composites, and the nanostructuring of these materials in polymers for structural and energy generation and storage applications. He is also co-founder and Chief Scientist of XG Sciences, Inc., a Michigan-based start-up company to produce graphene nanoplatelets. Specific ongoing projects include:
    - **Investigation into the enhancement of polymers with graphene nanoplatelets.** The objective of this project is to develop the next generation of aerospace structural multifunctional materials (polymer + fiber + nano particle) that will provide a balance between processing and performance. It is envisioned that an aerospace polymer composite compound will be developed which is modified.
with graphene nanoplatelets at various concentrations to provide a material optimized for: (1) strength and modulus, (2) electrical conductivity, (3) thermal conductivity, and (4) thermal expansion. This will involve extrusion processing and nanostructuring of the nanoparticles into highly aligned films for integration into composites.

**Nano-structured materials for Li ion battery and supercapacitors.** The objective of this research project is to: (1) gain a fundamental understanding of the atomic and molecular level processes that govern the operation, performance and failure mechanisms of energy storage systems; (2) design and investigate nanostructured materials with the goal of increasing the performance, durability and reliability of batteries and supercapacitors; (3) explore nanostructuring of materials for battery and supercapacitor materials to facilitate fast electron and ion transport with an emphasis on high-power and high-capacity batteries for electric vehicles.

Drzal’s portion of the project involves the nano-structuring of graphene nanoplatelets in the anode to improve capacity, re-charging rate and durability.

**Multifunctional composite materials.** The objectives of the research are: (1) to demonstrate a new approach to improving composite fracture and impact toughness by surface modification and coating with functionalized elastomeric coatings of nanoparticles and (2) to impart flammability improvement and flame resistance by the incorporation of xGnP into structural composite materials. The primary focus is on glass and carbon fiber reinforced vinyl ester composites used as structural elements in Army ground vehicles. The insertion of xGnP nanoparticles around fibers and between lamina in a composite can deflect blast and impact energy laterally away from the impact point and provide a safety margin by preventing structural collapse.

### RECENT PUBLICATIONS


Philip Eisenlohr  
Associate Professor  
eisenlohr@egr.msu.edu  |  517.432.4506  |  428 S. Shaw Lane, Room 3520

- **RESEARCH INTERESTS**
  Deformation mechanisms of crystalline solids, multi-physics simulation of microstructure mechanics

- **LAB**
  Computational Materials Mechanics (Engineering Bldg., 428 S. Shaw Lane, Room 1105)

- **WEBSITE**
  compmatermech.wordpress.com

- **GROUP MEMBERS**
  PHD STUDENTS: Eureka Pai Kulyadi and Ruxin Zhang  
  UNDERGRADUATE: Kyle Henrikson

- **CURRENT RESEARCH**
  *Computational prediction of advanced structural material performance by considering interactions of microstructure and plasticity in crystalline solids.* In our daily life, we heavily rely on the mechanical capacity and integrity of many different materials. For most structural materials of technological relevance, the mechanical behavior is intricately influenced by their chemistry (alloying in the case of metals) but even more importantly, by their microstructure. The latter is strongly impacted by processing conditions and, hence, can be substantially manipulated through processing. This complexity makes the prediction of the (thermo-) mechanical behavior of existing materials and the design of new materials and their required microstructures for targeted properties a remarkable challenge that is addressed at the Computational Materials Mechanics (CMM) lab by Eisenlohr and his group. We tap into the resources offered by the High Performance Computing Center (HPCC) and the Division of Engineering Computing Services (DECS) to simulate material deformation with commercial and homemade open-source software. In our simulations, we investigate the mechanisms of deformation occurring at mesosopic scales and connect them to the material microstructure. By this we seek, for instance, to (1) understand basic aspects of plastic deformation in crystals, (2) identify critical configurations in polycrystals or multiphase materials that might trigger nucleation of internal damage, and (3) predict the inherently anisotropic behavior of structural materials with complex microstructure at the scale of engineering components.

As an overarching theme, we seek to advance the forward modeling and associated simulation methodologies necessary to understand the properties of materials with (complex) microstructure and by that facilitate the solution of the inverse problem posed by the search for a microstructure that meets a given property demand.

A current example of ongoing research is: *Identifying the origins of whisker formation in tin films.* The spontaneous growth of tin (Sn) whiskers from tin coatings, which are frequently used due to their favorable properties such as excellent solderability, ductility, electrical conductivity, and corrosion resistance, is a serious concern to the electronic industry as these long filament-like structures pose a major risk of short-circuiting. Especially after lead (Pb), an alloying element that previously suppressed whisker growth, was banned in consumer electronics due to environmental hazards, understanding and mitigating whisker formation is of renewed interest. Current models of whisker formation simplify the film geometry into one dimension, partly consider plastic relaxation mechanisms, prescribe the stress condition surrounding a predetermined whisker grain, and are fitted to reproduce observed whisker growth rates. Yet none of those models can be regarded as predictive, since many open and critical aspects of whisker formation are not explicitly addressed by them. First and

![Figure 1](image-url)  
**Figure 1.** Spatial variability of hydrostatic stress $p$ in the vicinity of grain boundaries at three different film depth (surface to substrate from left to right). Substrate is not shown while part of the columnar grain structure of the tin film is illustrated at the far back and is colored according to the crystallographic direction that is parallel to the surface normal (close to $(100)$ in this example, see color code in standard stereographic triangle).
foremost, the specific conditions that trigger particular grains to grow a whisker are ignored and cannot be deduced from the simulation results. Secondly, the long-range stress gradient that is predicted to develop around a whisker grain has not been observed in highly resolved x-ray diffraction studies. Moreover, geometrically simplified models disregard the elastic and plastic anisotropy of Sn, hence, cannot account for measured influences of the global grain orientation distribution (crystallographic texture) on whisker propensity. Since whisker nucleation is ultimately a local phenomenon, specifics of the whisker grain neighborhood in terms of geometry and crystal orientations are very likely decisive factors.

We perform thermo-mechanically coupled full-field crystal plasticity simulations of tin films on an isotropic rigid substrate to investigate the influence of crystallographic texture, grain size distribution, and presence of oblique grains on the development of hydrostatic stress within the film, in particular within the network of grain boundaries, as that is the path for atom redistribution considered to be ultimately decisive for whisker formation. The exemplary results illustrated in Figures 1 and 2 demonstrate that a highly fluctuating hydrostatic stress field emerges under thermal strain that is influenced by the texture but essentially independent of the grain size distribution or the presence of non-columnar grain shapes. The results are consistent with the hypothesis that a whisker nucleates where low compressive stress relative to its immediate grain neighborhood occurs, a condition that appears to be predominantly determined by the crystallographic orientation distribution of the film.

**RECENT PUBLICATIONS**


**RESEARCH INTERESTS**
Energy, materials, sustainability

**LAB**
Fang Research Group
Engineering Bldg., 428 S. Shaw Lane, Room 3150

**WEBSITE**
https://www.fanggroup.org/

**SPECIAL EQUIPMENT AVAILABLE**
A dry room for solid-state battery materials processing; Cryogenic transmission electron microscopy (cryo-TEM) and cryogenic focused ion beam scanning electron microscopy (cryo-FIB-SEM) for electron-beam sensitive materials study; Titration Gas Chromatography (TGC) for trace metal quantification.

**GROUP MEMBERS**
UNDERGRADUATE STUDENTS: Megan Giltmier
COLLABORATORS: General Motors

**RECENT ACHIEVEMENTS**
Materials Research Society Graduate Student Award, 2019
Best Presentation, 2019 MRS Fall Meeting & Exhibit, 2019
Best Elevator Pitch Presenter, UCSD Sustainable Power and Energy Center Research Summit, 2019
Best Poster, 4th Lithium Battery International Summit, 2019

**CURRENT RESEARCH**
Our research interests cover different energy storage chemistry for various application scenarios, including, but not limited to, metal batteries (Li, Na, etc), all-solid-state batteries, multivalent-ion batteries and so on.

Our research is at the core of materials science by bridging concepts from analytical chemistry and electrochemistry, and hold technological prospects in multiple engineering disciplines, including two primary directions:

1. Developing multi-scale quantitative characterization tools, to answer key scientific questions in energy and environment related fields.

2. Developing new materials, precision fabrication/manufacturing methods, and system integration, guided by the fundamental understanding from quantitative characterization to manipulate molecular interactions at dynamic interfaces and innovate sustainable technologies.

**Anode-Free Lithium Metal Batteries:** In commercial lithium-ion batteries, lithium containing cathode provides the capacity, while graphite anode only serves as a host of lithium ions for safety considerations. Getting rid of the graphite anode, also called anode-free lithium metal battery (AFLMB), opens the opportunity to achieve a cell level energy density of 500 wh/kg and higher. The essence of AFLMB is to enable dendrite-free and high-efficient electrochemical cycling of lithium metal, requiring synergistic efforts of novel electrolyte design (both solid and liquid), fundamental understanding of lithium electrochemical behavior and system integration.¹

**Characterization by Design:** Titration Gas Chromatography (TGC): Inactive or “dead” Li formation is the immediate cause of capacity loss and safety hazards of high-energy lithium metal batteries; it consists of both (electro)chemically formed Li⁺ compounds in the solid electrolyte interphase (SEI) and electrically isolated unreacted metallic Li. However, quantitatively distinguishing between Li⁺ in SEI components and the unreacted metallic Li has not been possible due to the lack of effective diagnosis tools. We established a new analytical method, TGC, and accurately quantified the contribution from unreacted metallic Li to the total amount of inactive Li. We identify the unreacted metallic Li, rather than the (electro)chemically formed Li⁺ in SEI, as the dominant source of inactive Li and capacity loss.²

**Cryogenic Transmission Electron Microscopy (Cryo-TEM)** is a powerful tool to probe the nanostructures of electrochemically active materials, such as lithium metal and its SEI. It is impossible to acquire high-resolution images of these materials at room temperature due to their extremely sensitive nature to electron beam. The cryogenic protection minimizes the beam damage to the brittle materials while preserve its intrinsic properties.³
Cryogenic Focused Ion Beam (Cryo-FIB): FIB-SEM images provide the cross-section morphology information of materials. Cryogenic protection is critical because the electrochemically active materials are not only sensitive to electron beam, but also is apt to react with the FIB incident ion beam at room temperature. Taking a series of cross-sectional FIB-SEM images, a 3D structure can be reconstructed, enabling 3D visualization and quantitative structural analysis.4

**Materials by Design:** Surface Modification: Graphene oxide/polydopamine-coated Si nanocomposite (GO/PDA-Si) was synthesized by a novel facile solution-based chemical method at room temperature. The surface property of Si nanoparticles (NPs) was modified by introducing secondary amine groups from PDA, which form amide groups with carboxyl groups and hydrogen bonds with hydroxyl/carboxyl groups on GO. These chemical interactions firmly anchor Si NPs to GO so that aggregation of Si NPs can be mostly prevented.5

**Bulk Doping:** Oxygen-redox reactions in lithium-rich layered oxide cathode materials enable ultra high capacity, but causes voltage decay due to the unwanted oxygen gas formation. We firstly synthesized Li[Li0.2Ni0.2Mn0.6]O2 cathode materials by the modified co-precipitation method. Guided by the ab initio calculations of oxygen vacancy formation energy, we then selectively chose the Co and Mo co-doping into the Li[Li0.2Ni0.2Mn0.6]O2 materials with the aims to facilitate oxygen activity while mitigate the formation energy, we then selectively chose the Co and Mo

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**RECENT PUBLICATIONS**


C. Fang, X. Wang, Y. S. Meng, "Key issues hindering a practical lithium-metal battery", Trends in Chemistry, 1, 152-158. (2019)


Y. Shi, M. Zhang, C. Fang and Y.S. Meng, "Urea-based hydrothermal synthesis of LiNi0.5Co0.2Mn0.3O2 cathode material for Li-ion battery", Journal of Power Sources, 2018, 394, 114-121. (2018)


Robert C. Ferrier, Jr.
Assistant Professor
ferrier5@msu.edu | 517.884.7936 | 469 Wilson Road, Room 302A

- **RESEARCH INTERESTS**
  Polymer Chemistry, Polymer Physics, Nanocomposites, Materials Science.

- **LAB**
  Polymer Engineering Lab
  469 Wilson Road, Room 302A

- **WEBSITE**
  https://www.egr.msu.edu/ferrierlab

- **SPECIAL EQUIPMENT AVAILABLE**
  Malvern Omnisec GPC with Tetra-Detection, Nitrogen Glovebox, Schlenk Lines.

- **GROUP MEMBERS**
  Dr. Geetanjali Shukla, Niloofar Safaie, Shaylynn Crum, Gouree Kumbhar, and Mayson Whipple

- **PATENTS**

- **CURRENT RESEARCH**

  **Overview:** My group takes a holistic approach to polymer materials development. We start by developing new chemical methods to produce polymers with controlled structure, architecture, and chemistry. We then seek to understand the structure-property relationships of synthesized polymeric materials. We apply this knowledge to engineering materials for the broad areas of energy, environment, and health. Figure 1 is an overview of the work in our lab. Currently, we have several projects that are on-going and they can be broadly sorted into three different categories: (1) fundamental polymer chemistry / materials development, (2) charged polymers for energy and environment applications, and (3) polymers for biomedical applications.

  **Polymer Chemistry / Materials Development:** 2020 marked the 100th anniversary of Staudinger’s theory of the macromolecular nature of polymers. The last century of research and innovation on polymeric materials has sparked significant improvements to the quality of life of the average person, decreased production costs on consumer goods, and led to high-tech advances in the broad areas of energy, environment, and health. Despite the ubiquity of polymers, they are not a technological panacea and new polymeric materials, with unique and/or optimized properties, must be developed in order to further technology. Additionally, significant issues due to polymer waste have come to a head. Therefore, new polymerization methods need to be developed with a focus on new materials / properties and sustainability. To accomplish this, we have focused on synthetic techniques that combine monomers of disparate chemistries in new ways using earth-abundant aluminum compounds as our catalysts and initiators. Figure 2 consists of synthetic schemes for polyether (co)polymers with controlled end group and composition. Figure 3 shows kinetic and molecular weight characterization that we employ to optimize our polymeric materials.

  **Charged Polymers for Energy and Environment:** The interactions that govern the self-assembly of charged polymers, polyelectrolytes, have received wide-spread interest due to their prevalence in nature. For instance, charged amino acids in protein sequences allow for proper folding to accomplish cellular function. Charged proteins like aquaporin allow for controlled water transport through a membrane. Synthetic charged polymers have been utilized for applications in anti-fouling, encapsulation, separations, and ion transport. In my lab, we have focus on leveraging the unique characteristics of polyethers (e.g., backbone flexibility, ionic interaction), and the robust chemistry our aluminum based polymer synthesis method provides to
explore fundamental interactions between charged polymers as well as improve properties (e.g., ion transport) of these polymers for specific applications.

**Polymers for Biomedical Applications:** The opioid epidemic has claimed the lives of nearly half a million people in the USA between 1999 and 2018. Over-use of these powerful analgesics in a clinical setting has led to addiction to and abuse of illicit opiates like heroin. The increased accessibility to ever more powerful opiates has increased the overdose rate over the past few years. My lab is currently interested in utilizing novel polyether materials, or PEG-derivatives, to combat this issue. Our research in this area is nascent, but is focused on developing broad spectrum vaccines to substances of abuse to both help those with substance abused disorders and to protect first responders that may come into incidental contact with these substances. Our expertise is in quantum simulations, Materials by Design, Multiscale Simulations, Big Data, Machine Learning and Quantum Computing Algorithms.

![Figure 2](image1.png)  
**Figure 2.** Facile synthesis of (co)polyethers with compositional and end group control through a tunable aluminum initiator / catalyst system.

![Figure 3](image2.png)  
**Figure 3.** Top: Kinetics characterization of epoxide polymerizations. Kinetics can be tuned through catalyst concentration and chemistry. Bottom: Polymer molecular weight control.

### RECENT PUBLICATIONS

Assaf A. Gilad  
Professor of Chemical Engineering & Materials Science, Radiology and Neuroscience  
gilad@msu.edu  |  517.884-7468  |  775 Woodlot Dr., Room 2314

- **RESEARCH INTERESTS**  
  Evolution of genetically encoded sensors and activators for neuromodulation and biomedical imaging

- **LAB**  
  Institute for Quantitative Health Science and Engineering, 2300 Bio Engineering Facility, (775 Woodlot Dr) Room 2314

- **WEBSITE**  
  http://giladlab.iq.msu.edu

- **SPECIAL EQUIPMENT AVAILABLE**  
  https://gitlab.msu.edu/gilad-lab

- **GROUP MEMBERS**  
  **POSTGRADUATE FELLOW:** Nir Dayan, PhD  
  **GRADUATE STUDENTS:** Everett Baxter, Alex Bricco, Alejandro Castellanos, Joelle Eaves, Connor Grady, and Harvey Lee  
  **UNDERGRADUATE RESEARCH ASSISTANTS:** Katie Krell, Kylie Maxton and Adriana Wittke  
  **GILAD LAB STAFF:** Gabriela Saldana (Laboratory Technician/Manager), Adam Fillion (Laboratory Technologist), Allie Lapan (Laboratory Technologist), Brianna Ricker (Laboratory Technologist), and Rita Martin (Laboratory Administrator)

- **RECENT PUBLICATIONS**
  
  
  Bricco AR, Miralavvykomsari I, Bo S, Perlman O, Farrar CT, McMahon MT, Banzhaf W, Gilad AA. “Protein Optimization Evolving Tool (POET) based on Genetic Programming,” bioRxiv 2022.03.05.483103; doi: https://doi.org/10.1101/2022.03.05.483103. (2022)
  


- **PATENTS**
  
  
  
  
CURRENT RESEARCH

Recent advancements in DNA technologies allow scientists to develop new technologies based on “biological tools”. Those “biological tools” are at the foundation of a new field known as Synthetic Biology. Our lab is using this approach to tackle unmet needs in the biomedical field. Here we list few aspects of those challenges and their solutions.

**Diagnostics.** We have developed a family of genes that when expressed in cells can make those cells visible with magnetic resonance imaging (MRI). This technology is critical for monitoring the precision of cutting-edge therapeutics such as gene, stem cells and immunotherapy. We are developing Machine Learning tools for protein evolution in order to improve the sensitivity of these genes.

**Therapeutics:** We bioengineered a novel technology to remotely activate enzymes. We created an adaptation on the split protein method – where a protein is split into two parts that upon stimulation come together to create a functional enzyme - and utilize magnetic fields as the stimulus for activation. We use a magnetic perceptive protein, derived from the glass catfish (Kryptopterus vitreolus), as a “biomagnetic switch” that is controlled remotely by magnetic fields.

We have deployed this approach, termed magnetogenetics, to activate enzymes in E. coli and mammalian cells. We have created split NanoLuc, a split Peroxidase and a split Herpes Simplex Virus type 1-Thymidine Kinase (HSV1-TK).

**Bioremediation:** We developed biosynthetic technology to mitigate the rising concerns of medical pollution. This technology can reverse the long-term harmful effects of gadolinium-based MRI contrast agents on the wastewater, crops and living organisms.

**Neuroimaging:** We have developed a genetically encoded sensor for the neurotransmitter glutamate. This sensor is based on bioluminescence enzymatic reaction that allows an unprecedented depth of imaging. Inspired by marine organisms and evolution, our goal is to develop the next generation of genetically encoded technologies to solve urgent problems in the biomedical field.

**FIGURE 1.** In nature, proteins have evolved to perform extreme functions such as bioluminescence (generating light through enzymatic reaction; left) or sensing electromagnetic fields (as in the fish Kryptopterus vitreolus; middle). In the lab, we seek those genes and clone them to make the next generation of therapeutic and diagnostic technologies (such as MRI; right).
RESEARCH INTERESTS
Energy storage, electrocatalysis, biosensors.

LAB
Trout Food Science & Human Nutrition Building
469 Wilson Road, Room 301

WEBSITE
hickeylab.org

SPECIAL EQUIPMENT AVAILABLE
OLIS Rapid Stopped-Flow RSM 1000 spectrophotometer,
OLIS CLARITY 1000A Integrating Cavity (DSPC)
Spectroelectrochemical Cell.

GROUP MEMBERS
GRADUATE STUDENTS: Chase Bruggeman, Nunzio Carducci,
Sunanda Dey, Lincoln Mtemeri, and Sharmila Samaroo
UNDERGRADUATES: Abdullah Alahmad, Macy McPherson,
Jana Ratzloff, and Laina Young

CURRENT RESEARCH
The Hickey Group is focused on the design of electroactive
small molecules and polymer materials for a variety
of applications related to energy storage, catalysis,
and biosensing. Our research applies newly developed
electrochemical synthesis methodologies in creative ways to
solve research challenges. Furthermore, we aim to elucidate
electrochemical mechanisms and understand molecular
interactions at electrode interfaces. These interfaces are
vital for the development of next-generation technologies
to address global problems ranging from large scale energy
storage to the sequestration of greenhouse gases.

Recycling organic electrolytes for sustainable grid-
scale energy storage. Solar and wind power generation
technologies create a pathway towards minimizing
greenhouse gas emissions; however, the intermittent nature
of their power generation threatens grid stability. Redox
flow batteries (RFBs) could solve the problem of large-scale
energy storage. Unlike traditional batteries for which the
charge carrier and electrode are intrinsically coupled, RFBs
employ a liquid electrolyte charge carrier that can be flowed
over two oppositely polarized electrodes. This generates
an oxidized (catholyte) and reduced (anolyte) species that
are subsequently stored in separate holding tanks. By
decoupling electrolyte storage from the charge/discharge
electrode interface, it is possible to scale this energy storage
device as needed by simply increasing the storage tank
volume. The Hickey Group is focused on developing highly
stable anolytes and catholytes that can be produced at scale.

Low-cost enzymatic reactors through electrocatalytic
coenzyme regeneration. Nicotinamide adenine dinucleotide
(NADH) is perhaps the most ubiquitous coenzyme on the
planet, as it is utilized by >20% of all known enzymes.
Conversion of CO2 to propylene (so-called air to fuel),
N2 to ammonia (BioHaber-Bosch), and alkane activation
(drug synthesis) are among the many reactions catalyzed
by NADH-dependent enzymes at room temperature
and under mild aqueous conditions. Unfortunately, the

FIGURE 1. Schematic describing the use of an electrode stack
both for charging/discharging redox flow battery electrolytes
and electrochemically regenerating them from their decomposition products.

FIGURE 2. Structural comparison of natural nicotinamide adenine
dinucleotide (NADH) and artificial NADH biomimetics. Cyclic
voltammetry analysis used to elucidate electrochemical
reactivity of NADH biomimetics.
price of NADH (~$3,000 per mole) and lack of efficient regeneration methods renders NADH-dependent enzymes cost prohibitive on an industrial scale. To overcome this limitation, the Hickey Group is engineering small molecules from low-cost commodity chemicals that mimic the role of NADH for a chosen redox enzyme. Utilizing modular design strategies, we are tuning NADH biomimetics to enable catalytic recycling via simple electrochemical methods; thereby allowing us to use catalytic amounts of the artificial coenzymes in scaled enzymatic reactors.

**Enabling continuous monitoring of clinical analyte panels via peptide-based reagentless biosensor arrays.** For many complex diseases, no single diagnostic biomarker exists. Machine learning technologies and metabolomics studies have identified several biomarkers that, when taken together, may differentiate patients with early stages of aggressive disease from healthy individuals. However, validation and utilization of these predictive diagnostic models requires cost-effective population-scale biomarker screening tools are needed.

The Hickey and Woldring Groups are collaborating to develop modular electrochemical biosensors capable of simultaneously monitoring a panel of biomarkers in real-time to advance in-home disease screening, treatment, and monitoring.

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**RECENT PUBLICATIONS**


RESEARCH INTERESTS
Polymer composites processing and rheology

LAB
Polymer Processing and Rheology (Engineering Bldg., 428 S. Shaw Lane, Room 4155)

WEBSITE
http://www.chems.msu.edu/groups/jay/

SPECIAL EQUIPMENT AVAILABLE
Polylabs Torque Rheometer with a Banbury mixer attachment, Brabender drive with mini-Banbury mixer, Batch foaming apparatus, Solid-phase die-drawing apparatus, Dynisco capillary rheometer.

GROUP MEMBERS
PhD Students: Xing Lu and Swayam Shree.
Recent PhD Graduates: Christopher Hershey (Oak Ridge National Lab, Knoxville, TN), Xinting Lin (BASF, Ludwigshafen, Germany)

RECENT PATENTS

RECENT ACHIEVEMENTS
MTRAC Applied Advanced Materials awarded project: Additives and Polyolefin Blends for Automotive Bumper Fascias

CURRENT RESEARCH
The primary focus of current research in the Jayaraman lab is polymer composites processing and rheology.

Composite Tooling from Additive Manufacturing.
Development of lightweight, lower-cost tooling manufactured from advanced thermoplastic composites by additive manufacturing, to replace metal molds, has great potential in the automotive and aerospace industries.

The purpose of the current project is to examine the effect of uniform print orientation during mold manufacture, on its performance in molding operations. Mating mold halves were machined from a block of composite that was printed by extrusion deposition so that fiber orientation throughout the mold was along the closing direction of a press; this allowed for higher performance along the press closing direction -- higher thermal conductivity, higher stiffness as well as lower coefficient of thermal expansion (CTE) to be obtained along the press direction.

The thermal history of both the mold and the part during cure and the distortion of the molded part was predicted with the help of PAM-COMPOSITE software from ESI, Inc. The measured angle of the inclined surface in experimental molded parts was found to be close to the angle predicted by the software. Further development of predictive tools for the performance of tooling made with a variety of viscoelastic composites is underway.

FIGURE 1. (TOP) The smaller and lighter 3D printed composite tool mounted in the press. (BOTTOM) The part molded using the composite tool.
**Barrier Films with Balanced In-Plane Properties.** Layered silicates present interaction sites at both faces and edges of the nanolayers and silane coupling agents that locate at both sites lead to polymer nanocomposites with superior melt strength and properties. 1 mil thick films were prepared by film blowing and by biaxial stretching of extruded sheets from polypropylene copolymer nanocomposites with such coupling. The nanocomposite film exhibited balanced mechanical properties—tensile modulus, tensile strength and elongation to failure—along the draw direction and the transverse direction, in contrast to the properties for the neat PP copolymer film which were highly unbalanced. In addition, the permeability to gases and water vapor was reduced by half.

These trends may be understood in terms of the crystalline lamellar orientation distribution in the films. For example, FESEM images revealed that cross-hatched lamellae were absent from the unfilled PP blown film and were pervasive in the nanocomposite blown film. The nanolayers were oriented in the film plane with the longer dimension largely along the MD. The lamellar morphology of the polymer matrix in such films is being studied further with the help of SAXS.

**FIGURE 2.** The tensile modulus and elongation to break were significantly better along both directions in the plane of the film for nanocomposite blown films than for the matrix polypropylene copolymer film. The nanocomposite blown films are located closer to the diagonal, indicating greater isotropy in the film plane.

(TOP) The 1% secant modulus along the transverse direction (TD) plotted against the 1% secant modulus along the draw direction (MD), for the polypropylene copolymer PPC300 and three nanocomposites PPNC1 (5 wt%), PPNC2 (8 wt%) and PPNC3 (8 wt%).

(BOTTOM) The elongation to break along TD plotted against the elongation to break along MD, for the polypropylene copolymer PPC300 and three nanocomposites PPNC1 (5 wt%), PPNC2 (8 wt%) and PPNC3 (8 wt%).

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**RECENT PUBLICATIONS**


RESEARCH INTERESTS
Advanced materials and electroanalytical methods for energy conversion and storage technologies

LAB
Advanced Energy Materials Lab

WEBSITE
http://weilaigroup.org

GROUP MEMBERS
GRADUATE STUDENTS: Jin Dai and Yining He
CO-ADvised GRADUATE STUDENT: Tobias Glossmann (Oakland University)
UNDERGRADS: Sydney Boeberitz, Yalun Cai, and Dong Feng

CURRENT RESEARCH
Research interests in our lab have been broadly focused on the study of advanced materials and electroanalytical methods for energy conversion and storage technologies. Recently our research effort has centered around Solid-state Ionic Conductors (SIC) and Solid-state Mixed Ionic and Electronic Conductors (SMIEC) as battery electrolytes/electrodes and thermoelectric (TE) materials. SIC, SMIEC, and TE compounds are all complex materials with a framework-guest structure and unique ionic and electronic properties. The guest atoms in SIC and SMIEC are able to diffuse or conduct, while the framework is insulating (SIC) or semiconducting (SMIEC) for electrons, respectively. The guest atoms in TE are rattlers while the framework is semiconducting for electrons. The complexity of these materials calls for techniques known to both crystallographers and non-crystallographers. We are applying a suite of average and local structure and dynamics probes to understand their fundamental structure-property relationships.

Ongoing projects include:

Structure and dynamics of lithium-stuffed garnet oxides. State-of-the-art Li-ion batteries utilize organic solvent based liquid electrolytes that usually have limited electrochemical stability and are also volatile and flammable. Lithium-stuffed garnet oxides are a new class of nonflammable solid electrolytes with high lithium ionic conductivities. The framework of the materials is composed of LaO$_8$ dodecahedra and TaO$_8$ octahedra. There are two types of cages, tetrahedral (Td) and octahedral (Oh), to host lithium ions. Each Td cage is surrounded by four Oh cages and each Oh cage is surrounded by two Td cages. Both the Td and Oh cages are only partially occupied. We are investigating a prototypic series of lithium-stuffed garnet oxides Li$_{7-x}$La$_3$Zr$_{2-x}$Ta$_x$O$_{12}$ (x = 0–2). The scientific goal is to understand structure and dynamics of lithium disorder in these complex materials. Funding: National Science Foundation.

Structure and dynamics of thermoelectric materials. Currently around two-thirds of energy produced in US is rejected mainly in the form of waste heat. Such unused heat can be recovered by thermoelectric processes that...
directly convert thermal energy into electricity. Robust and cost-effective thermoelectric devices could have significant impact on the energy production and utilization of the society. Tetrahedrites are a class of TE materials based on Cu\textsubscript{12}Sb\textsubscript{4}S\textsubscript{13} containing earth-abundant and environmentally friendly elements. The structure consists of a 3D framework of CuS\textsubscript{4} tetrahedra and SbS\textsubscript{3} polyhedra. Another type of Cu atoms (Cu\textsubscript{12e}) behave as rattling guests inside a cage formed by three S and two Sb atoms. The interaction between Cu\textsubscript{12e} and Sb atoms is mitigated by the Sb lone pairs. We are currently investigating the relationship between atomic and electronic structure and thermoelectric properties of undoped and doped Cu\textsubscript{12}Sb\textsubscript{4}S\textsubscript{13} tetrahedrites. FUNDING: National Science Foundation.

**Bi-functional** electrode materials for Na-ion batteries. While Li-ion batteries have dominated the portable electronics market and started their penetration into the transportation and stationary markets, there is growing concern over the lithium abundance and geographical constraints of lithium minerals. Sodium element is more than 1000 times more abundant than lithium in earth’s crust and sea and sodium resources are considered practically unlimited. We are studying a class of sodium mixed oxides, Na\textsubscript{x}Ni\textsuperscript{x}Ti\textsubscript{1-x}O\textsubscript{2}, that have both high redox-potential transition metals, e.g. Ni, and low redox-potential transition metals, e.g., Ti. This suggests that these materials can be either utilized as a cathode or an anode, i.e., “bi-functional.”

**RECENT PUBLICATIONS**


M.J. Klenk, W. Lai, “Effect of exchange-correlation functionals on the density functional theory simulation of phase transformation of fast-ion conductors: A case study in the Li garnet oxide Li\textsubscript{7}La\textsubscript{3}Zr\textsubscript{2}O\textsubscript{12},” *Computational Materials Science* 134, 132–136 (2017).


Andre Lee
Associate Professor
leea@egr.msu.edu  |  517.355.5112  |  428 S. Shaw Lane, Room 3514

- **RESEARCH INTERESTS**
  Electronic packaging materials, solidification of materials, high-temperature polymers and their composites, phase, and synchrotron characterization

- **LAB**
  Inorganic-Organic Synthesis and Processing (3545 Engineering Bldg.)

- **SPECIAL EQUIPMENT AVAILABLE**
  Confocal Raman spectrometer with environmental control deformation chamber, high-pressure differential scanning calorimeter, rheometer, dynamic solid analyzer

- **GROUP MEMBERS**
  UNDERGRADUATE STUDENTS: Eric Egedy, Risa Hocking
  PHD STUDENTS: Tyler Johnson and Aditya Patil
  COLLABORATING FACULTY: Prof. Robert Maleczka (Chemistry)

- **PATENTS**

- **CURRENT RESEARCH**

**Electrochemical behavior of Cu-Al intermetallics in Cu wire bonding packages.** Wire bonding is a key packaging technology to achieve the electrical and mechanical interconnections between integrated circuit and the metal frame in printed circuit board. Recently, copper (Cu) has gained popularity over gold (Au) as the wire material based on cost reduction and higher performance. Two major intermetallics (IMCs), β (CuAl2) and γ (Cu4Al9), are often found in the Cu-Al bonding interface after the as-bonded structure undergoes thermal aging for extended periods of time. Galvanic corrosion for this Cu/γ/β/Al metallic-intermetallic “sandwich” structure, may take place when dissimilar metals are brought into electrical contact in the presence of an electrolyte containing corrosive species. In the service environment, moisture absorbed by the molding compound can dissolve a small amount of halogens (Cl–, Br–) used in the synthesis of molding compound and act as the electrolyte to initiate galvanic corrosion. Several studies have reported that the mechanical failure resulted from the disappearance of γ and failure occurred at the wire side. The use of Pd-coated Cu wire had shown to enhanced service reliability. It was suggested that the enhanced service reliability maybe due to the nobility of Pd addition, however, no systematic electrochemical characterization has been carried out for each of the entities in Cu(Pd)-Al bonding interface, which is essential to understand corrosion behavior of Cu(Pd)-Al bonding interface.

Using open circuit potentials and potentiodynamic polarization measurements systemic investigate were performed on all the undoped/Pd-doped samples (Cu, γ, θ) in different pH, Cl− concentration and temperatures to provide a complete picture of electrochemical behavior needed to understand the service reliability of wire bonded electronic packages. Electrochemical characteristic of metals were examined using cathodic and anodic polarization curves. Both $E_{\text{cor}}$ and $i_{\text{cor}}$ are determined by the thermodynamics (reversible potentials: $E(M/M_0^\text{rev})$, $E(Q/\text{OH}^\text{rev})$) and kinetics (exchange current densities: $i_\text{ex}(M/M_0^\text{rev})$, $i_\text{ex}(Q/\text{OH}^\text{rev})$), Tafel constants) of the two half-cell reactions. The addition of Pd increases the cathodic current density by increasing the exchange current density for ORR, and reduces the anodic current density by the induced passivation. This upward shift on the cathodic polarization curve, as well as the downward shift on the anodic polarization curve, led to an increase in the value of $E_{\text{cor}}$. However, the change in the value of $i_{\text{cor}}$ depends on the relative amount of shift between cathodic and anodic polarization curves. As shown in Figure 1(a), the upward shift in the cathodic polarization curve was more than the downward shift in the anodic polarization, the value of $i_{\text{cor}}$ will increase, which meaning a faster rate of corrosion. This was the case when only small amounts of Pd addition in Cu.

**FIGURE 1.** Determination of $E_{\text{cor}}$ and $i_{\text{cor}}$ of $g$ using polarization curves. The addition of Pd causing an upward shift of the cathodic branch and a downward shift of anodic branch of the polarization curve, leading to changes in $E_{\text{cor}}$ and $i_{\text{cor}}$.  

[Image of polarization curves]
To reduce the value of $i_{corr}$, it was necessary that the amount of downward shift be greater than the amount of upward shift, Figure 1(b). Therefore, a higher amount of Pd was needed to reduce the corrosion rate.

**Influence of nano-structured silanols on the microstructure of Al-Si casting alloys.** Aluminum (Al) based casting alloys have been used as light-weighting materials in the automotive industry for decades. Further weight reduction has been introduced in the automotive body construction recently with the use of structural aluminum. However, without modification, most of Al casting alloys have poor ductility, and does not meet the structural application requirement, i.e., at least 12% elongation to failure. Although, the addition of Na or Sr can spheroidize Si cuboids, and the addition of Ti and B reduce the grain size of primary aluminum phase in Al-Si based casting alloys. However, these modifications had some drawbacks needed to overcome, such as coarsening with aging as well as fading with repeated melting. Polyhedral oligomeric silsequioxanes (POSS) are silsequioxane-based nano-structural chemicals. These chemicals are cage like structures with repeated monomer units of $\text{RSiO}^{1.5}$ where Si is the element silicon, O is oxygen and R is hydrocarbon group, e.g., ethyl, isobutyl, phenyl etc. Partial cage-like POSS have the thermal stability in the molten aluminum and the silanol (Si-OH) functionalities form thermodynamically stable Si-O-M bonds with metals (e.g., Al). These nano-sized silanol compounds provide nucleation sites during solidification as grain refiner, and also serve as obstacles for preventing coarsening at elevated temperatures for microstructural stability of Al alloys.

A4047 and A4047 powders with and without POSS trisilanol added were used to make ingots for metallographic study. Figure 2 shows the optical micrographs of the ingots made of 325 mesh A4047 powders without and with POSS trisilanol addition, respectively. A4047 has a near-eutectic Al-Si composition with primary Al phase and eutectic Si-Al phase. Figure 2 (left) displays the microstructure of A4047 without POSS trisilanol, which is typical from a slow-cooled ingot with Al dendrite and lamellar Si cuboids. With the addition of POSS trisilanol, under the same casting and cooling configurations, the Si platelets are broken down to very fine spheroidized phase, as shown in Figure 2 (right).

The microstructure modification with POSS trisilanol added also leads to significant benefit in the mechanical property of A4047. Tensile tests were conducted on the tensile bars machined from the ingots. It was found that the elongation to failure had increased with POSS trisilanol addition, with percentage increase from 23% to 250% over the control sample (without POSS trisilanol added). In addition, the ultimate tensile strength did not decrease with the benefit of increases in the elongation to failure. Currently we are exploring different approaches for produce master alloys with different Si contents from hypoeutectic to hypereutectic Al-Si casting alloys.

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**RECENT PUBLICATIONS**

- L. Ma, Y. Zuo, S. Liu, F. Guo, A. Lee, K.N. Subramanian, “Whisker growth behaviors in POSS-silanol modified $\text{Sn}_{0.85}\text{Ag}_{0.15}\text{Cu}$ composite solders,” *Journal of Alloys and Compounds* 657, 400–407 (2016).
Ilsoon Lee
Associate Professor
leeil@egr.msu.edu | 517.355.9291 | 428 S. Shaw Lane, Room 1258

RESEARCH INTERESTS
Nanotechnology, polymers, adhesion, particles, biomimetics, self-assembly, nanomixing, nanodispersion, separation, renewable bioenergy, fluid flow

LAB
Polymer Surface, Interface, Nanotechnology Research Group (Engineering Bldg., 428 S. Shaw Lane, Room 2522)

WEBSITE
http://www.egr.msu.edu/~leeil/

SPECIAL EQUIPMENT AVAILABLE
Brookheaven ZetaPALS dynamic light scattering particle size analyzer/zeta potential analyzer; Primix TK Filmix ultra high-speed, thin-film mixer designed to produce stable nanodispersions; fluorescent and phase contrast optical micrographs with a digital camera connected to a computer (Nikon Eclipse ME 600 and ME 400 microscopes); layer-by-layer assembly and microcontact printing facilities; programmable slide stainer (Zeiss), spin coater, centrifuge, plasma cleaner (Harrick)

GROUP MEMBERS
Dr. Joung Sook Hong, Brooke Meharg, Chris Tawfik, Jing Yu

PATENTS

RECENT ACHIEVEMENTS
The poster “Development of Layered Multi-scale Porous Thin Films by Tuning Deposition Time and Molecular Weight of Polyelectrolytes” by J. Yu, O. Sanyal, A.P. Izbicki, I. Lee won the First-Place Poster Award ($500) in the Materials Science and Engineering Division (MSED) at the AIChE 2015 Annual Meeting in Salt Lake City, UT (November 8–13, 2015).
Affordable production of cellulose nanowhiskers (MIIE); Solar-Bio-Nano Based Wastewater System for the Production of Energy and Potable Water (DOD- SERDP); Understanding and Modulation of Electrostatic and Hydrophobic Forces within; Plant Cell Walls to Facilitate Enzymatic Deconstruction and Conversion to Biofuels (NSF); Prevention of Bacterial Biofilm Formation on Surfaces (SPG).

CURRENT RESEARCH
Dr. Ilsoon Lee’s nano bio engineering laboratory is utilizing nanotechnology and self-assembly as new tools to design new nanostructured materials and systems to solve existing engineering problems in energy, materials, and environment. The research focuses on the design and fabrication of nano/bio particles and films to advance energy, biocatalytic systems, and functional materials.

Figure 1. This work focuses on the design of porous polymeric films with nano- and micro-sized pores existing in distinct zones.
Specific selective projects include:

- Prevention of bacterial biofilm formation on surfaces
- Solar-bio-nano based wastewater system for the production of energy and potable water
- Hybrid nanostructured metal foam material systems for blast impact (and wrinkle-free films)
- Fabrication of functional nanoparticles and delivery system
- Fast and efficient production of cellulose nanowhiskers and the use in the composite materials
- Understanding and modulational of interfacial properties within plant cell wall pores to facilitate enzymatic deconstruction and conversion to biofuels.

**FIGURE 2.** Perchlorate rejection enhanced by surface modification via LbL assembly technique. Optimized membrane had much higher permeability and equivalent rejection than RO.

**FIGURE 3.** Surfaces and interfaces capable of repelling, attracting, and selectively detecting molecules have attracted attention for their important application in catalysts, coatings, sensors, and devices, including biologically implantable ones.

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**RECENT PUBLICATIONS**


RESEARCH INTERESTS
Spectroscopic quantification and modeling of hydrogen-bonded systems; properties of bio-derived chemicals and fuels.

LABS & LOCATIONS
Properties Lab (Engineering Bldg., 428 S. Shaw Lane, Room 2255).

WEBSITE
https://www.egr.msu.edu/thermoprops/

SPECIAL EQUIPMENT AVAILABLE
Vapor-liquid equilibria measurements, flash point, cloud point, densitometry, low- and high-pressure speed-of-sound, IR and NMR measurements of hydrogen bonding.

GROUP MEMBERS
Bill Killian, Renming Liu, Andrew Norfleet, Lars Peereboom

RECENT PATENTS


CURRENT RESEARCH
The Lira Thermodynamics Research Facility measures and correlates vapor-liquid equilibria (VLE), liquid-liquid equilibria (LLE), and solid-liquid equilibria. For VLE, the lab has a Fisher T-xy recirculating apparatus, a custom P-xy apparatus, and a miniature ebulliometer. We also have capabilities for density and viscosity measurements.

A new modeling approach. Separation operations are generally the most expensive components of chemical processes. Therefore, it is especially important to optimize separations to accelerate the concept-to-implementation timeline of a project. Designing these operations requires accurate and flexible thermodynamic models, but existing tools often fall short when applied to systems with polar components. The hydrogen bonding which occurs between these components has a dramatic effect on chemical properties and the phenomenon is poorly represented in traditional models. This work aims to address this limitation by: (1) developing a thermodynamic model which incorporates a statistical mechanics approach (Wertheim’s perturbation theory) to calculate the extent and effects of association; (2) evaluating parameters for the model by leveraging a combination of IR and NMR spectroscopy as well as molecular and quantum simulations; and (3) delivering the resulting model as a commercial tool (an Aspen Plus user model) to be utilized by industrial partners and the broader engineering community.

Activity coefficient models permit accurate fitting of pure component vapor pressures independently of mixture parameters, but traditionally the models don’t represent association effects of hydrogen bonding. Adding the Wertheim association term addresses the deficiency. The approach adds the association term to the typical residual and combinatorial terms,

\[ \ln \gamma = \ln \gamma_{\text{res}} + \ln \gamma_{\text{com}} + \ln \gamma_{\text{assoc}} \]

Figure 1 shows the improvement for the methanol + cyclohexane system compared to the traditional NRTL.

Quantum mechanics to guide spectroscopy. A unique feature of the MSU associating fluid project is the incorporation of quantum calculations to guide interpretation of the spectra in collaboration with Professor James Jackson in the Chemistry Department. Our dedicated 28 supercomputer cores with 512 GB RAM on the MSU Institute for Cyber-Enabled Computing permit us to run quantum calculations on medium-sized clusters. In our approach, we run molecular simulations (MD) to generate realistic molecular environments and save frames. We minimize the hydroxyl and nearby atoms using quantum mechanical (QM) PM6 and then run minimization and frequency calculations at the B3LYP/6-31G* level of theory.

Figure 2 shows that the attenuation coefficient for absorption of radiation changes significantly with the
bonding of hydrogen for n-butanol in cyclohexane. The same pattern holds whether the vibrations are coupled or uncoupled. From the clusters we identify bonding motifs as shown by the inset of Figure 3. In literature, the infrared absorbance peak at 3640 cm\(^{-1}\) has been speculated to be both alpha and beta hydroxyls. Our calculations confirm the empirical assumptions. The gamma hydroxyls vibrate at intermediate frequencies and absorb more strongly. The delta bonds vibrate at lower wavenumbers and absorb very strongly, as shown by large absorption coefficient in Figure 2 below 3350 cm\(^{-1}\). However, some configurations have opposing dipole configurations which cancel absorption, resulting in a constant attenuation function in that range. We have developed the empirical attenuation coefficient function shown by the right axis as inspired by the Haan mean of the quantum calculations.

**Spectroscopic determination of association.** We use the attenuation coefficient function to scale the experimental spectra by dividing the cleaned spectra absorption by the attenuation function as shown by the example spectra in Figure 3. After scaling, the integrated area is linear with concentration and independent of temperature as expected by Beer’s law. This is the first time that temperature-independent quantification of the hydroxyl peak has been obtained. Figure 3 illustrates curve fitting, where each curve represents a different bond type. The \(\alpha\) and \(\beta\) represent unbounded vibrational contributions are the peak to the left. Using the MD/QM results as a guide, we assign vibrational frequencies ranges to the type of bonds shown in Figure 3 inset as \(\alpha, \beta, \gamma, \delta\). By curve fitting the scaled spectra, we obtain populations of the different bond types and we can fit the bond distribution with an engineering model as shown in Figure 4 where the bond distributions as a function of concentration are represented in this figure with two parameters. By collecting spectra at various temperatures, we are incorporating the bond distribution into the thermodynamic model as a function of temperature and concentration.

**Figure 2.** Extinction coefficients as a function of the hydrogen-bonding classification and the wavenumber as predicted by the B3LYP/6-31G* level of theory for n-butanol in cyclohexane. The molar attenuation coefficient line is inspired by the Haan mean of the MD/QM results and has been adjusted to spectroscopic data.

**Figure 3.** Illustration of curve fitting for quantification of bond types. The spectra is scaled using the function from Figure 2 after removing the solvent contributions. The peak locations correspond to the bond types as suggested by quantum calculations.

**Figure 4.** Fit of the hydrogen bond distribution for n-butanol in cyclohexane (solid lines) compared to spectroscopic data. The dashed lines are the bond distribution as calculated by the Gross/Sadowski parameters.

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**RECENT PUBLICATIONS**


**RESEARCH INTERESTS**
Organic and molecular electronics, quantum dots, renewable energy, solar cells, light-emitting diodes, excitonic photo-physics, crystal growth, molecular therapeutics and imaging

**LAB**
Molecular and Organic Excitonics Laboratory

**WEBSITE**
http://www.egr.msu.edu/~rlunt/

**SPECIAL EQUIPMENT AVAILABLE**
Thin film device fabrication, characterization, and testing; in situ diffraction; ellipsometry; luminescence spectroscopy

**GROUP MEMBERS**
GRADUATE STUDENTS: Matthew Bates, Chris Herrera, Aungkan Sen, Chenchen Yang

**RECENT ACHIEVEMENTS**
2019: Associate Editor, Science Advances, AAAS
2017: Outstanding Faculty Award, Awarded by the Senior Class Council, MSU
2016: Johansen Crosby Endowed Chair
2016: Withrow Distinguished Junior Scholar Award
2016: MSU Teacher Scholar Award
2015: Top Innovators Under 35 List, MIT Technology Review
2015: Ovshinsky Sustainable Energy Fellowship Award, American Physical Society (APS)
2015: MSU Undergraduate Research Faculty Mentor of the Year Award
2015: MSU Innovation of the Year Award
2013: DuPont Young Professor Award
2013: NSF CAREER Award

**CURRENT RESEARCH**
The Molecular and Organic Excitonics (MOE) laboratory focuses on excitonic and nanostructured materials relevant in four thrust areas: (1) energy production, (2) energy storage, (3) energy utilization, and (4) therapeutics. We aim to synthesize and exploit oriented, crystalline, nanostructured, and excitonic thin film semiconductors through organic-inorganic and organic-organic interactions while studying fundamental relationships between growth, structure, and photophysical properties. We look to apply this understanding to enhance device performance and create unique electronic functionality.

**Routes to lower cost solar cells through nanostructured and excitonic materials.** The Earth is continuously bathing in over one-hundred-million-billion watts of sunlight ~ several thousand times more than mankind’s energy demands. While a multifaceted approach is required to transition away from fossil fuels, solar energy will surely be key to a sustainable future. The engineering of PV structures at the nanoscale has attracted research interest as it may enable substantial reductions in PV installation costs and facilitate wider market penetration. Ultimately we aim to further evaluate and exploit these new materials in thin-film architectures to realize ubiquitous and low-cost solar energy.

**Excitons for building integrated transparent PVs and solar concentrators.** We are pioneering transparent molecular photovoltaics that can retain a high degree of visible-transparency, while absorbing ultra-violet and near-infrared light for power generation. These cells can allow for optimization of overall transparency, efficiency, and lighting aesthetic and lead to a highly deployable solar window that is retrofittable in window panes in homes, skyscrapers, airports, greenhouses, malls, and automobiles, and enhance the functionality of already utilized transparent surfaces. This is accomplished by exploiting the excitonic character of molecular and organic semiconductors that leads to “oscillator bunching” exhibiting uniquely distinct absorption spectra from the band-absorption of traditional inorganic semiconductors.

**RECENT PATENTS**
“Gallium indium nitride nanocrystals,” (provisional patent filed Sept., 2019.)
“Near-infrared harvesting transparent luminescent solar concentrators with engineered stokes shifts,” (provisional patent filed May 2018.)
“Flexible inorganic perovskite solar cells and room-temperature processing thereof,” (provisional patent filed 2018.)

![FIGURE 1. LEFT: High-light of our work on the cover of Adv Optical Materials showing a photograph of the pioneering transparent luminescent solar concentrator (LSC) system that selectively harvests infrared light. RIGHT: Diagram of excitonic molecules for these transparent concentrators (top) and the demonstrated quantum efficiency in the infrared (bottom).](image-url)
Next-generation organic light emitting diodes for lighting. An important route to the reduction of green gasses lies in energy utilization. In particular, lighting accounts for about 17% of the total energy consumption in buildings. State of the art white organic light emitting diodes (WOLEDs) are currently poised to make reductions in this consumption rate for lighting as power efficiencies greater than that of fluorescent lighting have been demonstrated. However, WOLEDs are currently limited by external quantum efficiencies (EQE) of ~20% due to waveguided modes and are reliant on precious metal (Pt and Ir) containing phosphorescent dopants. To circumvent these shortcomings we are designing the next-generation devices based on phosphorescent nanostructured and abundant molecular materials.

Understanding organic epitaxy. The presence of excitons in organic semiconductors at room temperature distinguish them from traditional semiconductors, providing exceptional opportunities for manipulating energy in a range of structures from light emitting diodes, lasers, transparent photovoltaics, and optical switches. However, control over crystalline order, orientation, and defect formation are crucial to the fabrication and optimization of these excitonic electronics. The overarching goal of understanding organic epitaxy is to explore bottom-up vapor-deposition routes to the growth of large-area organic and molecular crystalline films with enhanced properties.

**RECENT PUBLICATIONS**


Ilce G. Medina-Meza  
Assistant Professor  
ilce@msu.edu | 517.884.1971 | 469 Wilson Rd. Room 302C

- **RESEARCH INTERESTS**
  Translational chemical biology and engineering, lipidomics, metabolomics and processomics systems biology.

- **LAB LOCATION**
  **Food and Health Engineering Lab**
  Michigan State University
  Trout Food Science & Human Nutrition Building
  469 Wilson Road, Room 305

- **WEBSITE**
  https://www.egr.msu.edu/ilcehealth/

- **SPECIAL EQUIPMENT AVAILABLE**
  GC-MS, GC-FID, HPLC, nitrogen evaporator multi-vap

- **GROUP MEMBERS**
  Anam Hasem, (Visitor Scholar), Aline DaSilva, (Postdoctoral Research); Lisaura Maldonado-Pereira, (Graduate Student)
  Undergraduate Research Assistants: Grant Gmitter, Ashley Xu, and Lisa Zhou

- **CURRENT RESEARCH**
  The Medina research laboratory focuses on translational chemical biology and engineering using a cutting edge multiomics-based systems biology approach for metabolic biomarker discovery. The laboratory combines high-throughput screening measurements, in vitro and biomimetic assays, mass spectrometry-based metabolomics/lipidomics and predictive kinetic modeling to obtain a better mechanistic understanding of the role that food metabolome plays in many biological processes, including oxidative stress, inflammation, and chronic diseases.
  In this context, we have identified candidate cholesterol and lipid-derived metabolites that are being validated in clinical studies as biomarkers in cardiovascular and neurological disorders associated with oxidative stress. Additionally, the chemical analysis of the metabolome in human biofluids and tissues provides a wealth of information on human health, including the assessment of disease state and diagnosis, drug targets and toxicity. By performing a metabolite fingerprinting, new discoveries linking cellular pathways to biological mechanisms are being revealed and shaping our understanding of cell biology, physiology, and medicine.

**FIGURE 1.** Food and Health Engineering landscape, underlying different model systems to evaluate the oxidative stress biomarkers.
Lipid oxidative stress represents one of the major issues in chronic diseases, including neurological and cardiovascular pathologies. These potentially harmful oxidative species can be generated in vivo, or can be introduced by diet, especially in high-fat nutritional diets such as in Western developed countries.

The lab’s research embraces the study of these oxidative molecules in a broader way, going from their occurrence in food matrices to metabolomics principles applied in biological systems, like cell tissues and lipoproteins (Figure 1).

We are challenging the limitations of the current approaches by i) investigating chemical and physical mechanisms that trigger oxidative stress during food processing and handling, ii) mapping lipid and cholesterol oxidation products in the US diet, and iii) looking for potential biomarkers of oxidative stress in vivo and ex vivo systems. This is achieved by state-of-the-art analytical means, supported by engineering and statistical tools, like kinetic modeling and high-order statistical analyses.

Our research has impact in several fields, including food processing and safety, nutrition, as well as broader biomedical significance. We are actively collaborating with clinicians and researchers across the US, including MSU Medical School, DeVos Hospital, Michigan Alzheimer’s Disease Center and George Washington University.

**RECENT PUBLICATIONS**


RESEARCH INTERESTS
Computational materials science; quantum and atomistic simulations; machine learning, scientific computing. Energy/Materials: 2D-materials; energetic materials; catalysis; beyond-Li ion batteries; fuel cells; polymers; artificial photosynthesis.

LAB
Materials, Processes and Quantum Simulation Center (MUSIC) Lab
428 S. Shaw Lane, Room 1105

WEBSITE
https://www.egr.msu.edu/~jmendoza/

SPECIAL EQUIPMENT AVAILABLE
Dedicated computer clusters at the MSU High Performance Computing Center, state-of-the-art GPUs and workstations.

GROUP MEMBERS
William Comaskey, Marcus Djokic, Yu-Hsiu Lin, Daniel Maldonado, Austin Rodriguez, Sean Stafford.
RECENT ALUMNI: Srimanta Pakhira (Professor at Indian Institute of Technology); Carlos Aguirre (Professor at National Polytechnic Institute/IPN); N. Abdulrahman (Research Associate at Brookhaven National Laboratory); Valdirio Segundo (Engineer at Engenharia e Analista de PI); Eric Rubiel (Data Scientist at Machine Learning Startup); Austin Eovito (Data Scientist at IBM); Andy Murray (Product Physicist at Sun Nuclear Corporation); Sarah Palmon (Grad at Rice University); Rosemary Bier (Engineer at Geosyntec Consultants); Marlon Facey (Software Engineer at Google); Sachin Kamiya (Trader at Bank of America Merrill Lynch); Finn Carlsvi (Engineer at Google X); Alexander Aduenko (Machine Learning at Finance - WorldQuant); Alex Anemogiannis (Data Scientist at Uhana); Yubo Su (Grad at Cornell); Alan Menezes (GPU Architect at NVIDIA); Amanda Rees (founder at Bold).

CURRENT RESEARCH
My research focuses on the development and application of numerical techniques to study structural, electronic, transport and optical properties of materials, low-dimensional systems and nanostructures. Computer simulations performed in my group have addressed physical and chemical properties of 2D-materials, porous materials, catalysts, nanotubes, polymers, catalytic/metallic/magnetic clusters and molecular machines.

The problems we study are studied require developing or expanding established methods related to: Multiscale - Multiparadigm simulations: Quantum Mechanics (DFT, CCSD), Atomistic Simulations (MD, Force Field development, ReaxFF, Coarse grained FF), Statistical Mechanics and Computational Engineering (Chemical Engineering and...
RECENT PUBLICATIONS


Mendoza-Cortes, J. “Controlling catalytic reactions for production of hydrogen (HER), fuel cells (ORR), and carbon dioxide reduction (CO2RR),” in Abstract of Papers of the American Chemical Society vol. 257 (2019).
Donald Morelli
Professor
dmorelli@egr.msu.edu | 517.432.5453 | 428 S. Shaw Lane, Room 2100

RESEARCH INTERESTS
Materials physics, new semiconductors for energy applications, thermal and electronic transport in solids

LAB
Electronic Materials Laboratory (Engineering Research Complex, 1497 Engineering Research Court, Room E172)

WEBSITE
www.egr.msu.edu/morelli-research

SPECIAL EQUIPMENT AVAILABLE
Equipment for synthesis of materials, including vacuum melting, arc-melting, and powder processing; x-ray diffractometer for crystal structure and phase identification; electrical and thermal transport property characterization from 80–1000K

GROUP MEMBER
Corey Cooling

CURRENT RESEARCH
Research in the Morelli group is aimed at designing, synthesizing, and characterizing new inorganic materials with applications in energy conversion. Currently, two main thrusts or our research are (1) investigation of new thermoelectric materials for conversion of heat to electricity; and (2) development of new materials for cryogenic cooling of Peltier devices for space-based applications.

The Center for Revolutionary Materials for Solid State Energy Conversion, a US Department of Energy–funded research center led by MSU, focuses on solid state conversion of thermal energy to useful electrical power, both to increase the efficiency of traditional industrial energy processes and to tap new unused sources of energy such as solar thermal. Additionally materials with enhanced thermoelectric properties will find application in high efficiency, environmentally benign climate control systems. We are undertaking a broad-based effort in semiconductor energy conversion materials utilizing and combining experimental, theoretical, and computational efforts. A major focus of our effort will be in the synthesis of new forms of matter, including both single phase alloys and compounds and composite structures created using nanoscience.

Ultimately, by working together in this Center we aim to develop design rules to predict properties of advanced thermoelectric materials, and realize these structures through innovative synthesis and advanced structural as well as chemical characterization.

Some examples of current work in our group include the following:

Understanding the relationship between structure and bonding and the thermal conductivity of solids. Good thermoelectric materials have very low thermal conductivity, and if we can understand how to control this parameter, new materials can be designed with improved properties. In collaboration with colleagues in our Center, we have combined state-of-the-art computational approaches with thermal and electronic transport characterization to study the relationship between crystal structure and properties of a class of promising semiconductors (Figure 1). We find that certain types of structural arrangements of atoms give rise to strongly anharmonic lattice vibrations, a key ingredient in determining a material’s heat conduction characteristics. We have synthesized these predicted structures in the laboratory and verified the predictions of these computational models.

Thermoelectric materials synthesized from earth-abundant sources. We have shown that the mineral tetrahedrite (Figure 2) can be used directly as a thermoelectric material with very little compositional modification. Tetrahedrite, of chemical formula Cu$_{12}$Sb$_4$S$_{13}$, is the most common sulfosalt mineral on Earth, and its use as a source thermoelectric material could pave the way to large scale and low cost application of thermoelectricity for energy conversion. We have found that the mineral itself can be used directly in a powder processing methodology to synthesize materials with large thermoelectric figure of merit in a temperature

FIGURE 1. Structural sub-units in the thermoelectric compound tetrahedrite. The structure is characterized by (a) tetrahedrally coordinated Cu (1); (b) trigonally coordinated Cu(2); (c) tetrahedrally coordinated S(1); (d) octahedrally coordinated S(2); (e) trigonally coordinated Sb. Electronic and thermal transport properties are determined by the detailed nature of structure and bonding in this material.

FIGURE 2. Tetrahedrite, of chemical formula Cu$_{12}$Sb$_4$S$_{13}$, is the most common sulfosalt mineral on Earth, and its use as a source thermoelectric material could pave the way to large scale and low cost application of thermoelectricity for energy conversion.
Recent Publications


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**Figure 2.** A natural mineral tetrahedrite polycrystal (left). This compound is the most widespread sulfosalt on earth; it is also a semiconductor whose properties can be tailored to produce high thermoelectric figure of merit. The crystal structure of this compound is shown on the right.

Range suitable for the conversion of waste heat from a variety of sources, including vehicle exhaust gas and power plant discharge sources.

**Thermoelectrics for cooling of infrared sensors.** Our group has also been investigating new materials for low temperature Peltier devices. These devices can be used to cool infrared sensors on satellites to the cryogenic temperatures necessary for them to operate. We are exploring thermoelectric effects below room temperature in alloys comprised of elements containing f-shell electrons. Two new compounds of particular interest are YbAl₂ and YbCu₂Si₂. We have found that by chemical substitution the magnitude of the Seebeck coefficient can be increased, and the temperature at which it is maximized can be controlled. This provides a means of improving and optimizing the thermoelectric properties in the cryogenic temperature range.
RESEARCH INTERESTS
Design and engineer biobased and biodegradable-compostable plastics, develop environmentally responsible end-of-life options for plastics and bioplastics materials, conduct carbon footprint and life cycle assessment (LCA) of materials, studies in reactive extrusion processing and biofiber composites

LAB
MBI, 3815 Technology Blvd., Lansing, MI

WEBSITE
www.msu.edu/~narayan

PATENT

GROUP MEMBERS
POSTDOCTORAL & VISITING RESEARCH FELLOWS: Professor Philippe Dubois (Univ. of Mons, Belgium), Dr. Elodie Hablot (Univ. of Strasbourg, France), Dr. Weipeng Liu (Green Star Company, China), Dr. Mohan Patil (UICT, India), Dr. Jean Marie (Ben) Raquez (Univ. of Mons, Belgium), Dr. Yuya Tachibana (AIST, Japan), Professor Y.Z. Wang (Sichuan Univ., China). STUDENTS: graduated 19 PhD and 20 Master’s students; currently 5 graduate students and 8 undergraduates work in the group.

CURRENT RESEARCH
Biobased Materials Research Group design and engineer new biobased and biodegradable-compostable polymer materials and bio processes using agricultural crops and residues (soybean and corn), lignocellulosic biomass, and algae. These biobased products find commercial application in films for plastic bags, injection molded articles, thermoformed products, foamed sheets for protective and insulation packaging, and The group’s biobased materials technology platform is covered by 29 patents; 200 peer reviewed publications, and several technologies have been licensed or resulted in a spin-off company. Successful technology commercialization exemplars are:

- poly(lactic acid) (PLA) technology—the world’s foremost 100% biobased and biodegradable-compostable material— with a 150,000-ton commercial plant operating in Blair, Nebraska, by NatureWorks LLC (www.natureworksllc.com)
- biopolyester and modified PLA resins for biodegradable-compostable films, molded products, and engineering plastics through Northern Technologies (www.natur-tec.com), a $150 million NASDAQ traded company
- biofoam sheet manufacturing for cushion and insulation packaging under the trade name GreenCell by KTM Industries (www.ktmindustries.com)
- biobased polyols technology for flexible and rigid polyurethanes in partnership with a Michigan agribusiness, Zeeland biobased products (www.zfsinc.com)
- licensing four patents on thermoplastic modified starch and its copolymers with biopolymesters to Ingredion Inc., a $2.3 billion international company.

The major R&D and technology commercialization effort underway is building an industrial soybean based biorefinery producing value added industrial products in Michigan in cooperation with Zeeland Farm Services (www.zfsinc.com). ZFS is Michigan’s largest soybean processor servicing about 2,500 Michigan farmers and processing 26,000 bushels of soybean (1.56 million pounds) per day—representing 99% of the soybeans grown in the state. Currently they produce two products namely soybean meal used as animal feed, and oil which is used in food applications. Diversifying the product base with higher value industrial products provides more economic stability and job creation to the Michigan economy. We developed an ozonolysis technology platform to convert the fatty acid methyl esters derived from soybean oil to C-9 diesters and C-9, C-7 monoesters which have industrial applications. The
plant oils are being converted into biobased polyols which is used in making flexible polyurethanes for automotive and industrial applications.

The soy meal residue remaining after removing the oil by solvent extraction is rich in proteins and carbohydrates. We are developing technology to make rigid polyurethane foams. Figure 2 shows samples: A is reference formulation with no soy polyol; B contains 25%, and C contains 50% of soy polyol. Another synthetic strategy being developed is to convert the soy meal to polyurethane building blocks by eliminating or reducing the use of the toxic isocyanate reagent.

Our biobased and biodegradable-compostable hybrid materials technology platform is based on poly(lactide) (PLA) resins derived from plant-biomass feedstock like corn and sugarcane. Funded by NSF SBIR Phase I and II grants, the technology is being commercialized by Natur-Tec, a business unit of Northern Technologies (NASDAQ: NTIC). The company currently supplies biodegradable-compostable bags to global companies such as Levi Strauss & Co. About 76,000 m.t./yr of plastic packaging resins are used for packaging 5 billion garments in South Asia alone (Figure 3), translating to about $200 million in economic value.

The group is working towards addressing the major issue of microplastics in the ocean environment. In a recent paper published in the journal Science (February 2015, 347:6223, 768), we reported that 4.8 to 12.7 million tons of plastics entered into the oceans in 2010 and without any intervention would increase to 10.4 to 27.7 million tons by 2025. The paper shows that reducing 85% of waste from the top 35 mismanaged waste countries would result in a 75% reduction of plastic waste going into the oceans. We are working towards developing and implementing compostable plastics technology in conjunction with composting and anaerobic digestion systems to prevent “mismanaged plastic waste” from entering into the oceans. These efforts along with along with educational and consumer awareness messaging can clearly advance the goal to “a cleaner ocean environment.”

**Recent Publications**


Jason D. Nicholas
Associate Professor and Materials Science Graduate Recruiting Coordinator
jdn@msu.edu | 517.355.1615 | 1449 Engineering Research Ct., Room C9C

- RESEARCH INTERESTS
  Solid state ionics, mechano-chemical coupling, solid oxide fuel cells, ceramic-metal joining, mineral physics

- LAB
  Solid State Ionics Laboratory (Energy and Automotive Research Laboratory, 1497 Engineering Research Court, Room 172)

- WEBSITE
  https://www.egr.msu.edu/nicholasgroup/

- SPECIAL EQUIPMENT AVAILABLE
  Thin film deposition, controlled atmosphere/high temperature wafer curvature measurement

- GROUP MEMBERS
  Genzhi Hu

- RECENT PATENTS

- RECENT ACHIEVEMENTS
  - Publication of the world’s most highly cited “ceria sintering aid” paper
  - Development of the world’s most highly cited nano-composite Solid Oxide Fuel Cell electrode model (the SIMPLE model)
  - Development of a new Ag-Ni stainless steel to ceramic brazing technique
  - Demonstration of how the mechanical response of multilayer samples can be used to simultaneously measure a variety thin film mechanical, thermal, and electrochemical materials properties in situ

- CURRENT RESEARCH
  Understanding the factors controlling ion surface exchange in electrochemical devices. Solid Oxide Fuel Cells (SOFCs) have energy densities five times higher than the world’s best battery, efficiencies three times higher than the world’s best internal combustion engine, and NOx and SOx emissions 100 times lower than conventional power plants. Unfortunately, widespread SOFC commercialization is limited by the high operating temperatures (> 600°C) required to incorporate oxygen into the device. Further, attempts to engineer the oxygen surface coefficient, \( k \), have been complicated by the large \( k \) discrepancies in the literature for nominally identical materials under nominally identical conditions (such as the 10,000 times discrepancy in the 650°C \( k \) of the model material \( \text{La}_{0.6}\text{Sr}_{0.4}\text{FeO}_3 \)).
  Recently, the Nicholas group developed a new in situ, non-contact, current collector-free wafer curvature technique that simultaneously measures the oxygen surface exchange coefficients and biaxial stress state of thin film oxygen reduction reaction (ORR) or oxygen evolution reaction (OER) catalysts. Further, the Nicholas Group demonstrated that some of the \( k \) variation in the literature is caused by Pt current collector enhancement and Si surface impurity impairment of the oxygen surface exchange reaction. The hypothesis of the present work is that differences in grain size, surface structure, and stress state are responsible for the rest of the \( k \) variation and can be used to tailor the performance of \( \text{La}_{0.6}\text{Sr}_{0.4}\text{FeO}_3 \). This will be evaluated by (1) performing curvature relaxation measurements on samples with varying grain sizes and intentionally varied surface structures, (2) comparing global \( k \) values from curvature relaxation to local \( k \) values from secondary ion mass spectroscopy depth profiling, and (3) comparing the observed behavior to density functional theory–based models. This work will hopefully lead to improved solid oxide fuel cell, solid oxide electrolysis cell, gas-sensing, catalytic converter, water splitting, water purification, and other ion-exchange-enabled devices.

**Thin film diamond anvil cell studies to determine how deviatoric stress alters subducting slab phase transformations.** The mechanism(s) responsible for deep focus earthquakes are important for understanding the dynamics of mantle convection, subduction, and seismic hazards within the Earth. Although multiple mechanisms have been proposed to explain the existence, frequency, and source characteristics of deep focus earthquakes, no one mechanism is consistent with all the observations. The objective of the present work is to evaluate the hypothesis that a combination of geologically-relevant deviatoric stresses, preferred crystallographic orientation, and/or new metastable phases stabilize the olivine-structured \( \text{Mg}_2\text{SiO}_4 \) found within subducting oceanic crust. This will be achieved by (1) using pulsed laser deposition to produce \( \text{Mg}_2\text{SiO}_4 \) thin films with intentionally varied crystallographic orientations,
grain sizes, and deviatoric stress levels, (2) using in situ wafer curvature measurements to measure the deviatoric stress in each thin film sample outside of a diamond anvil cell versus temperature, and (3) using externally heated diamond anvil cell thin film Raman spectroscopy to observe the impact deviatoric stress and temperature have on the kinetics and thermodynamics of the Mg$_2$SiO$_4$ olivine to spinel phase transformation. In addition to providing new insights into the mechanisms responsible for deep focus earthquakes, the techniques developed here will allow mineral physicists to perform optically-accessible experiments under previously inaccessible stress states, demonstrate a new class of thin film pressure sensors, and show how geologically relevant high-pressure phases can be stabilized in thin film form for use in everyday devices.

**High performance circuit pastes for solid oxide fuel cell applications.** SOFCs are a unique green technology capable of providing improved efficiencies for today’s hydrocarbon-based economy while also providing a pathway to a CO$_2$-neutral future. Unfortunately, SOFC circuit paste degradation and delamination, especially upon thermal and/or redox cycling, is a major problem that can shorten SOFC lifetimes. Recently the Nicholas Group discovered that porous nickel interlayers could be used to promote the wetting and spreading of silver on a variety of ceramic substrates.

The objective of the present work is to find ways to modify that approach to produce resilient silver-based electrical circuits. If successful, this work will result in a new, cost-effective class of thick-film circuit pastes with lower sheet resistance, lower contact resistance, better redox cycling stability, better rapid thermal cycling stability and better adhesion to a variety of SOFC materials than today’s best commercially available contact pastes.

**Degradation and performance studies of ald-stabilized nano-composite solid oxide fuel cell cathodes.** Nano-composite SOFC cathodes produced by the infiltration and subsequent firing of nitrate solutions exhibit excellent performance. Unfortunately, significant amounts of high temperature infiltrate particle coarsening results in unacceptably high nano-composite cathode degradation rates. The objective of the present work is to use atomic layer deposition (ALD) to stabilize the performance of La$_{0.6}$Sr$_{0.4}$Co$_{0.8}$Fe$_{0.2}$O$_{3-x}$-Ce$_{0.2}$Gd$_{0.8}$O$_{1.95-x}$ (LSCF-GDC) cathodes developed by the Nicholas Group and previously shown to exhibit the world’s best low-temperature SOFC cathode performance of ~0.1 Ω cm$^2$ at 550°C.

**Recent Publications**


RESEARCH INTERESTS
Transport phenomena (single phase and multiphase); rheology of suspensions, turbulent flows in rotating and nonrotating frames, hydrocyclone classifiers and separators, animal orientation and navigation, computational transport phenomena for undergraduates

CURRENT COLLABORATING STUDENTS
Andrew Bowden (Chemical Engineering, Undergraduate Professorial Assistant), Abdul Motin (PhD Candidate, Mechanical Engineering, A. Bénard, Advisor), Devinda Wijewardena (Chemical Engineering, Undergraduate Professorial Assistant).

CURRENT COLLABORATING FACULTY & COLLEAGUES
Dr. André Bénard (Mechanical Engineering, MSU), Dr. Farhad Jaberi (Mechanical Engineering, MSU), Dr. YoChan Kim (PhD 2006, MSU, Bechtel National), Dr. Karuna Koppula (PhD 2009, MSU, Rochester Institute of Technology), Dr. Vlad Tarabara (Environmental Engineering, MSU).

NSF INDUSTRY/UNIVERSITY COOPERATIVE RESEARCH CENTER, 2004–2011
C. Petty and A. Bénard, Founders and Co-Directors, Michigan State University, University of Tulsa, Central Florida University, University of Akron, Ansys, Bechtel, BP, CD-adapco, Chevron, ConocoPhillips, M-I Swaco, Petrobras, Pfizer, National Science Foundation, Department of Interior (MMS).

PATENT

CURRENT RESEARCH
Multiphase transport phenomena research and education. Multiphase fluids (i.e., drilling fluids, foodstuffs, pharmaceuticals, blood, liquid crystalline polymers, aerosols, fuel sprays, oil/water dispersions, solid/liquid suspensions, liquid/gas mists, and bubbly liquids) occur ubiquitously in many applications in engineering, polymer science, human medicine, and biology. Computational methods can provide significant insights related to the behavior of these fluids in extreme conditions and in complex geometries. Examples include hydrate formation in subsea pipelines; oil/water spills in the ocean; dust storms on Earth and on Mars; circulation of large scale ocean currents; mixing of pollutants in lakes and rivers; ice formation in the atmosphere; particle deposition in the lungs; and, effluent flows from hydrocyclone separators.

Flows of multiphase fluids are often unstable and involve large-scale secondary motions that can significantly influence multiphase mixing and separation, interfacial mass and heat transfer, and multiphase reactions. Professor Petty and his colleagues are interested in the further development and experimental validation of next generation multiphase transport phenomena closure models and the further development of computational transport phenomena methods for rapid analysis and design of processes with an emphasis on safety.

Turbulent fluctuations and bird navigation. The solution of the Reynolds-Averaged Navier-Stokes equation is the only viable means for simulating high Reynolds number flows typically encountered in engineering practice and in the troposphere. Research at MSU for the past 20 years has developed a realizable, algebraic Reynolds stress closure for rotating and nonrotating turbulent flows. The theory predicts the redistribution of turbulent kinetic energy among the three components of the velocity in simple mean shear flows (Figure 1). The new approach is being used to analyze atmospheric scintillation of electromagnetic waves induced by the local coupling between the angular velocity of Earth and fluctuations in the turbulent velocity field. The relationship between scintillation phenomena and bird migration may provide an explanation of a longstanding question in biology: How do birds navigate over global scales?

Cross flow filtration hydrocyclone for liquid/liquid separation. A cross flow filtration hydrocyclone (CFFH) combines the desirable attributes of a vortex separator and a filter. By selecting a hydrophilic filter medium, a CFFH clarifier has the potential to produce a filtrate phase

![Turbulent Energy Distribution](image-url)
with a low concentration of a dispersed organic phase in a single stage. The CFFH concept may provide a practical means to mitigate three problems associated with current hydrocyclone clarifiers: (1) the loss of separation performance due to core flow reversal; (2) the loss of separation performance due to entrained particles in the sidewall boundary layer; and, (3) the loss of separation performance due to turndown. The third feature may be the most significant inasmuch as the CFFH environment provides a self-regulating means to reduce the local filtrate flux across the sidewall filter. The CFFH concept for produced water can be extended to crude oil dehydration, to liquid/liquid separation of concentrated phases encountered in liquid/liquid extraction applications, and to downhole and subsea separation of oil and water. The objective of current research is to develop a prototype oil/water separator for field testing.

**Multiphase flows.** Particle-laden flows are widely encountered in the oil and gas industry. An accurate description of particle transport in turbulent flows is of great importance for predicting fouling of various equipment as well as erosion of pipe walls. As illustrated by the jet-pulsed mixer shown below (Figure 2) and flow through a bend (Figure 3), deposition of particles on the walls is influenced significantly by streamlines curvature of the flow field.

**FIGURE 2** (*right, top*). Path lines colored by axial velocity (m/s) at 5 seconds into Cycle 4 (suction phase). Note the toroidal secondary flows within the PJM as well as in the tank. (NSF/Combined Research and Curriculum Development Case Study. D. Eldein, S. Teich-McGoldrick, J. Roth, and C. Trainer. “CFD Simulation of a Pulsed-Jet Mixer,” Second Place Ribbon: Undergraduate Poster Session, Annual AIChE Meeting, 3–8 November 2002, Indianapolis, Indiana)

**FIGURE 3** (*right, bottom*). Flow patterns through a bend (180°) with cutouts that show various recirculation patterns at different cross-sections. The turbulence model and the wall functions strongly influence the qualitative accuracy of the simulation (P. Zhang, PhD, Mechanical Engineering, 2012, MSU).

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**RECENT PUBLICATIONS**


RESEARCH INTERESTS
Polymer engineering, biomimicry, interfacial engineering

LAB LOCATION
Engineering Bldg., 428 S. Shaw Lane, Room 2535

WEBSITE
https://carolineszczepanski.com

SPECIAL EQUIPMENT AVAILABLE
Dynamic mechanical analysis (DMA), goniometry (contact angle measurements and surface analysis), FTIR spectroscopy

GROUP MEMBERS
PhD STUDENTS: Sabrina Curley (MSE), Denghao Fu (MSE), Allie VanZanten (MSE), Ingrid Calvez (jointly-supervised with Université Laval)
UNDERGRADUATE STUDENTS: Emily England (MSE), Justin Hamlin (CHE), Alison Huckins (CHE), Walter Kretzer (CHE)

RECENT GRANTS

CURRENT RESEARCH
Our natural world is rich with materials having properties that are incredibly valuable for science and engineering applications. This includes plant surfaces such as the lotus leaf that can repel water, bones that can withstand the mechanical and bacterial stresses encountered in the human body, and the adhesive interfaces of mussels that function remarkably underwater. However, being unsustainable to harvest or isolate naturally occurring materials on a larger scale, a challenge is how to replicate this level of performance using elegant materials engineering. My research group confronts this challenge by taking advantage of natural designs via biomimicry, and letting natural inspiration motivate our technical innovations.

The overarching goal of the Szczepanski research group is to identify robust, versatile strategies to recreate complex material designs, utilizing polymer engineering. Research in our group develops materials for a variety of applications including biomaterials, coatings and adhesives:

Novel polymers for in vitro dental applications:
Photopolymerized composite restorations (e.g., fillings) are standard practice in clinical dentistry. Unfortunately, these synthetic materials fail at a higher rate than prior technologies, mainly, amalgam-based materials. This represents a major challenge in biomaterials and costs roughly $5 billion annually. My group confronts this challenge by designing novel polymer networks appropriate for dental restorative applications. This work is multifaceted, as we must address the current mechanical limitations of employed dental materials, while also mimicking the appearance, integrity, and performance of our native tooth structure.

Biomimetic Interfaces: Numerous natural systems have surface functionalities (e.g., fluid repellency, adhesion) that are of value and of interest to replicate for modern materials development. Unfortunately, a major challenge with employing biomimicry to recreate interfacial performance observed in nature is that it requires high precision in terms of surface chemistry and topography. Currently, chemical and/or topographical patterning is achieved via complex processing that is ill-suited for implementation outside of a research setting, and rarely are both surface chemistry and topography simultaneously addressed and tailored. To address this disconnect, multiple projects in my group investigate novel polymerization strategies to create intricate and elegant patterning of polymer interfaces, with an emphasis on approaches that are relevant for large scale production. As one example, micro and nanoscale surface topography significantly impacts interactions with light, and a matte appearance can be engineered via micro-structured roughness and surface topography. Through a collaboration with Prof. Véronic Landry (Université Laval, Canada), our group works on establishing effective strategies for self-matting coatings applied to wood interior products.

FIGURE 1: SEM images of topographical surface features generated via in situ photo- (top) and electro- (bottom) polymerizations.
**Bio-inspired and bio-sourced materials to tailor polymer composites and networks:** My research group has also made significant contributions in the growing use of bio-sourced materials for adhesive and composite applications, mainly using additives such as cellulose nanocrystals (CNCs). CNCs are an additive of interest as their crystalline nature can provide mechanical reinforcement and improve barrier performance of composites. Furthermore, being derived from natural feedstocks, CNCs are a promising renewable and sustainable material source. However, a challenge with employing CNCs as additives is establishing effective and uniform dispersion in a wide range of polymer matrices. Our ongoing work with CNCs addresses how composites and adhesives can be enhanced with this type of nanomaterial.

**RECENT PUBLICATIONS**


RESEARCH INTERESTS
Biomolecular engineering, novel therapeutics and diagnostics, persistence and success in engineering education

LAB
Applied Biomolecular Engineering Laboratory (Engineering Building, 428 S. Shaw Lane, Room 2125)

WEBSITE
https://www.egr.msu.edu/people/profile/spwalton

SPECIAL EQUIPMENT AVAILABLE
Fluorescent and chemiluminescent imaging, cell culture facilities

GROUP MEMBERS
GRADUATE STUDENTS: Kevin Chen, Chauncey Splichal.

RECENT GRANTS
NSF–ENG–EEC Research Initiation
“Understanding the Impact of Institutional Supports on the Motivation, Belonging, Identity Development, and Persistence of Engineering Students”
AWARD #1830269; p.i.: S. Patrick Walton; co-p.i.: Lisa Linnenbrink-Garcia; ORGANIZATION: Michigan State University; NSF ORGANIZATION: EEC; START DATE: 01/15/2019; AWARD AMOUNT: $210,000

CURRENT RESEARCH
Nucleic acid therapeutics are the next frontier in medicine. Clinical applications of small, interfering RNAs (siRNAs), antisense oligonucleotides, messenger RNAs, and CRISPR are realities. In therapeutics, nucleic acids are typically bound to or encapsulated in a delivery vehicle to protect the nucleic acids during transport to the target cells and to facilitate entry into the target cells. The Applied Biomolecular Engineering Laboratory (ABEL), led by S. Patrick Walton, is currently working to design nucleic acid-based therapeutics based on understanding their mechanism of action.

Recent efforts have focused on the mechanisms that cells use to take in material from outside the cell, endocytosis. By exposing cells to chemical inhibitors, we classified the endocytic pathways cells use to internalize siRNA complexes (Figure 1). Our work reinforces an essential consideration for design of nucleic acid-containing complexes: which pathway(s) to use and which to avoid in a given cell type to maximize siRNA function.

FIGURE 1: By blocking endocytic pathways using chemical inhibitors (e.g., Filipin), we can determine which pathways are important for the activity of siRNAs. siRNAs (red dots) are being delivered to reduce the expression of Green Fluorescent Protein.
After the material enters the cell, it is critical that it is transported to the proper intracellular locations where they can achieve function. To complement our endocytosis studies, we have developed an approach to analyze intracellular trafficking of nucleic acids (Figure 2). To develop the approach, we generated cells expressing the green fluorescent protein (GFP). Using these cells, we have preliminarily found that where siRNAs go in cells changes how they function.

In collaboration with colleagues from the College of Education, Dr. Walton is examining how to apply the science of motivation to better understand engineering student success. It is his goal to expand the research on engineering student success beyond the typical metrics of persistence and GPA. Dr. Walton’s research will examine student success by many metrics to help the broader engineering community better understand how to support students with different short and long-term ambitions, ultimately enhancing the diversity of individuals and skills in the engineering workforce.

**Figure 2:** Using genetic tools, we increased the expression of endocytic proteins to confirm the activity of the corresponding pathways in the activity of siRNAs.

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**RECENT PUBLICATIONS**


Daniel R. Woldring
Assistant Professor
woldring@egr.msu.edu | 517.353.2349 | 775 Woodlot Dr., Room 4116

- **RESEARCH INTERESTS**
  Therapeutics, diagnostics, drug discovery, protein engineering

- **LAB**
  Institute for Quantitative Health Science & Engineering - Woldring Lab (IQ Building, 775 Woodlot Dr., Room 4116)

- **WEBSITE**
  woldring.org/research/

- **GROUP MEMBERS**
  GRADUATE STUDENTS: Sunanda Dey, Ben Dolgikh, Mehrsa Mardikoraem, Sam Schmidt.
  UNDERGRADS: Theo Belecciu, Joelle Eaves, Claudia Kramer, Ashley Maloney, James VanAntwerp, Zirui Wang
  COLLABORATORS: Michael Bachmann, David Hickey, Masako Harada, Xuefei Huang, Jens Schmidt, Erik Shapiro.

- **PATENTS**

- **CURRENT RESEARCH**
  Developing high performance therapeutics and diagnostics using novel protein engineering methods. The Woldring lab focuses on the discovery and fundamental study of high-performance binding proteins having utility as precision medicines, disease diagnostic agents, and fundamental research probes.

  There is a critical need for such reagents that facilitate the detection and treatment of challenging diseases; however, the rate at which they are developed by the scientific community fails to meet this demand. To address this, our research combines the power of high-throughput yeast surface display selection methods with precise structural and dynamic information. We can then leverage simulations of protein interactions to empower a feedback loop between theory and experiment to elucidate protein evolution.

**FIGURE 1:** Therapeutics for COVID-19 are explored using computer simulations to engage functional components of SARS-CoV-2 (yellow ribbon) with numerous small molecule drugs (red, blue, green sticks). Lead candidates are identified by calculating the location and strength of binding interactions between the drugs and viral proteins.
Relevant Publications

**RECENT PUBLICATIONS**

- **Book Chapter Series within Methods in Molecular Biology, Yeast Surface Display edition 2021**, accepted:
  - B. Dolgikh and D.R. Woldring, “Site-wise diversification of combinatorial libraries using insights from structure guided stability calculations.”
  - J. VanAntwerp and D.R. Woldring, “Ancestral sequence reconstruction and alternate amino acid states guide protein library design.”


**Figure 2:** Protein engineering of chemical transporter proteins can allow for targeted delivery and regulation of immune cells to treat aggressive diseases. Identifying which regions of a transporter protein can be adjusted in order to change the overall function of the protein is an important step toward achieving clinical goals. Using statistical analysis among a large collection of related proteins from a diverse group of species can be used to locate the functionally important regions of these complex biomolecules.
R. Mark Worden
Professor
worden@egr.msu.edu | 517.353.9015 | 428 S. Shaw Lane, Room 2263

- **RESEARCH INTERESTS**
  Multiphase biocatalysis, nanobiotechnology, biomimetic interfaces, biosensors, bioelectronics

- **LAB**
  Nanobiotechnology and Biomimetic Interfaces (Engineering Bldg., 428 S. Shaw Lane, Room 2525)

- **WEBSITE**
  [http://www.chems.msu.edu/people/profile/worden?user=worden](http://www.chems.msu.edu/people/profile/worden?user=worden)

- **GROUP MEMBERS**
  Ziwei Wang

- **PATENTS**

- **CURRENT RESEARCH**
  **Multiphase biocatalysis.** Focus includes developing cost-effective and carbon-neutral methods to produce biofuels and chemicals from high-energy gases such as hydrogen and carbon monoxide. His group has been funded by the NSF and DOE to use microbubbles to enhance gas mass transfer. In a recent project funded by DOE’s ARPA-E Electrofuels program, Dr. Worden’s lab collaborated with the group of Dr. Anthony Sinskey at MIT to develop a bioprocess for continuous conversion of the gaseous reactants H₂, CO₂, and O₂ into the biofuel isobutanol (IBT). To address the three significant bioreactor-design challenges: (1) extremely high demands for gas mass transfer; (2) safety issues resulting from the simultaneous use of by H₂ and O₂ gases, which form explosive mixtures; and (3) biocatalyst inhibition by the IBT, Dr. Worden’s group developed a novel Bioreactor for Incompatible Gases (BIG). The BIG features a hollow fiber module that allows the H₂ and O₂ gases to be kept on opposite sides of the membrane and transferred to the cells without forming unsafe gas mixtures. In addition, product inhibition is controlled by continuous removal of the IBT as it is formed. A prototype bench-scale BIG has been assembled in a walk-in hood, and an automatic process control system has allowed the bioreactor stably for up to 19 days. These experiments have demonstrated for the first time continuous IBT production from H₂, CO₂, and O₂.

  **Nanobiotechnology and biomimetic interfaces.** This focus has recently been used to better understand cell toxicity caused by engineered nanomaterials (ENM). The approach uses an artificial bilayer lipid membrane (BLM) to mimic a cell membrane. When ENM interact with a BLM, pores are formed in the BLM, and the resulting leakage of ions through the pores can be measured. Dr. Worden’s group recently used electrochemical impedance spectroscopy provides a sensitive method to measure ENM’s potency in disrupting biomembranes. One study showed that the method could discern differences in the potency of polystyrene nanoparticles (PNP) having different in size and surface charge. Negatively charged, carboxyl modified PNP

**FIGURE 1.** Schematic diagram of nanoparticles (spheres) removing lipid molecules from a biomembrane (shown as a layer of lipid molecules on the gold electrode).
20 nm in diameter were more potent in disrupting BLM than those 100 nm PNP. However, positively charged amidine modified nanoparticles, 120 nm PNP were more potent than 23 nm PNP.

**Biosensors and bioelectronics.** This focus is exemplified by a project funded by the NSF Accelerating Innovation Research program to advance a biosensor patent toward commercialization. The project addresses the need for more high-performance, inexpensive biosensors able to detect toxic organophosphorus pesticides and nerve agents. The objectives are (1) to adapt the redox-cycling biosensor interface to nanoparticle-functionalized electrodes, (2) to develop a redox-cycling biosensor interface for alkaline-phosphatase-linked antibodies, and (3) to adapt redox-cycling biosensor interfaces to three commercial biosensor platforms. Conductive nanomaterials are being incorporated into the bioelectronic sensor interface and functionalized to measure activity of an organophosphate as an electric current. Additional bioelectronic sensors are also being developed that use a redox-recycling mechanism to amplify biosensor signals that measure binding of enzyme-linked antibodies to their target antigen. A portfolio of potentially commercializable prototype bioelectronic immunosensors is being developed in collaboration with an original equipment manufacturer.

Dr. Worden has been active in leveraging research in these areas to develop novel educational programs that integrate multidisciplinary research with pedagogy. He has served as PI on two grants by the Department of Education’s Graduate Assistance in Areas of National Need (GAANN) program to develop graduate Ph.D. training programs entitled, “Interdisciplinary Training Program on Bioelectronics” (seven co-Is) and “Multidisciplinary

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**RECENT PUBLICATIONS**


RESEARCH INTERESTS
Crystal growth; crystallography; thermal properties of materials, including thermal expansion, sound velocity, bond anharmonicity

LAB
Advanced Materials for Thermal Energy Conversion and Storage (Engineering Bldg., 428 S. Shaw Lane, Room 2530)

WEBSITE
https://alexzevalkink.wordpress.com
YouTube channel: “Zevalkink Research Group”

SPECIAL EQUIPMENT AVAILABLE
Optical floating zone furnace for crystal growth up to 2200°C; resonant ultrasound spectroscopy for measurement of elastic constants and sound velocity up to 500°C in controlled atmosphere; high-resolution, high-speed x-ray diffractometer with 2D pixel array detector, and high-temperature stage with controlled atmosphere up to 1400°C

GROUP MEMBERS
PHD STUDENTS: Mario Calderón, Sevan Chanakian, Ashiq Shawon, Towhidur Rahman, Monique Noel, Erik Vyhmeister-Cancel; POST-DOCTORAL RESEARCHER: Eleonora Isotta

RECENT GRANTS
NASA–JPL: High-temperature structure and bonding in Zintl thermoelectrics, $203,000, start date 01/08/18.
NSF–DMR SSCM, Traveling solvent crystal growth of anisotropic Zintl thermoelectrics, $328,750, start date 8/16/17, award #1709158

CURRENT RESEARCH
Our research leverages crystal growth and high-temperature characterization techniques to study the relationship between atomic structure, bonding and the electronic and thermal properties of functional materials. Ultimately, we aim to apply this understanding to engineer improved functional materials for energy applications. Our recent efforts have focused on crystal growth using optical floating zone, flux, and Bridgman methods, and on measurements of the high-temperature sound velocity and lattice expansion in materials used for thermoelectric energy conversion.

Crystal growth of anisotropic materials. Our current aim is to develop improved thermoelectric materials for use in radioisotope thermoelectric generators designed and tested at NASA’s Jet Propulsion Laboratory. The thermoelectric materials used in this application must be semiconductors with very high melting temperatures, optimized electronic properties, and low thermal conductivity. They must also be mechanically robust over a large temperature gradient.

Many candidate materials have atomic structures that are extremely anisotropic, and are therefore predicted to have more favorable electronic properties along specific crystal orientations, as illustrated in Figure 1 for Ca$_5$In$_2$Sb$_6$. This anisotropy is expected to lead to improved thermoelectric properties along the high conductivity direction. One of the most significant barriers, however, to understanding the intrinsic electronic and thermal properties of complex semiconductors is the scarcity of large single crystal samples. This is particularly limiting in the case of anisotropic materials, for which measurements of bulk, single crystalline samples yield only “averaged” properties.

In our laboratory, we are utilizing several high-temperature techniques to grow single crystals of semiconducting and ceramic materials from the melt. Our main focus is optical floating zone growth, illustrated in Figure 2, which is a powerful method for materials with very high melting temperatures and relatively low vapor pressures. An optical floating zone furnace consists of several halogen lamps set in elliptical mirrors (four, in our case). The mirrors focus the light on the center of the chamber, where two polycrystalline

FIGURE 1. SEM of Ca$_5$In$_2$Sb$_6$ crystals obtained from flux growth and (b) an example of the FIB cutting process used to extract individual micro-ribbons from the crystals. (c) A 3D rendering of the circuit design shows the Cr-Au sensors (yellow) deposited on top of both the sample (grey) and the glass substrate (blue). (d) SEM image of a Ca$_5$In$_2$Sb$_6$ micro-ribbon with final implementation of the circuit design.
rod-shaped samples are suspended inside of an inert gas-filled quartz tube. A stable “floating” molten zone is established where the two rods meet. During growth, both rods are moved downwards, so that the floating zone slowly progresses up the length of the feed rod. This method can also be adapted to materials with incongruent melting behavior by employing a molten flux (i.e., solvent material) instead of melting the target compound.

**Resonant ultrasound spectroscopy.** The thermal and elastic properties of materials are critical in a wide range of applications. Resonant ultrasound spectroscopy (RUS) is an elegant approach to characterize the elastic constants of bulk and single crystal samples by measuring the vibrational resonant frequencies. This method is also ideal for measuring the full elastic tensor of anisotropic single crystals, as the entire tensor is obtained in a single measurement. High-temperature RUS measurements coupled with high temperature x-ray diffraction—also available in our laboratory—gives us an extremely sensitive set of tools to investigate structural changes in materials, including gradual softening of bonds, order-disorder transitions, and structural phase changes.

**FIGURE 2.** (A) Screen-shot from the growth of a TiO₂ crystal using the optical floating zone method. (B) Schematic of the interior of a floating zone furnace showing the sample mounted inside of an evacuated quartz tube. Light from four halogen bulbs is focused on the center of the sample, creating a floating molten zone.

**FIGURE 3.** The resonant ultrasound method uses a piezoelectric transducer to emit acoustic waves over a range of frequencies. Certain frequencies will resonate strongly in the sample, yielding a vibrational response that is detected by a second transducer. This method allows us to study the elastic tensor of single crystals and polycrystalline materials at room temperature and at high temperatures.

**RECENT PUBLICATIONS**


