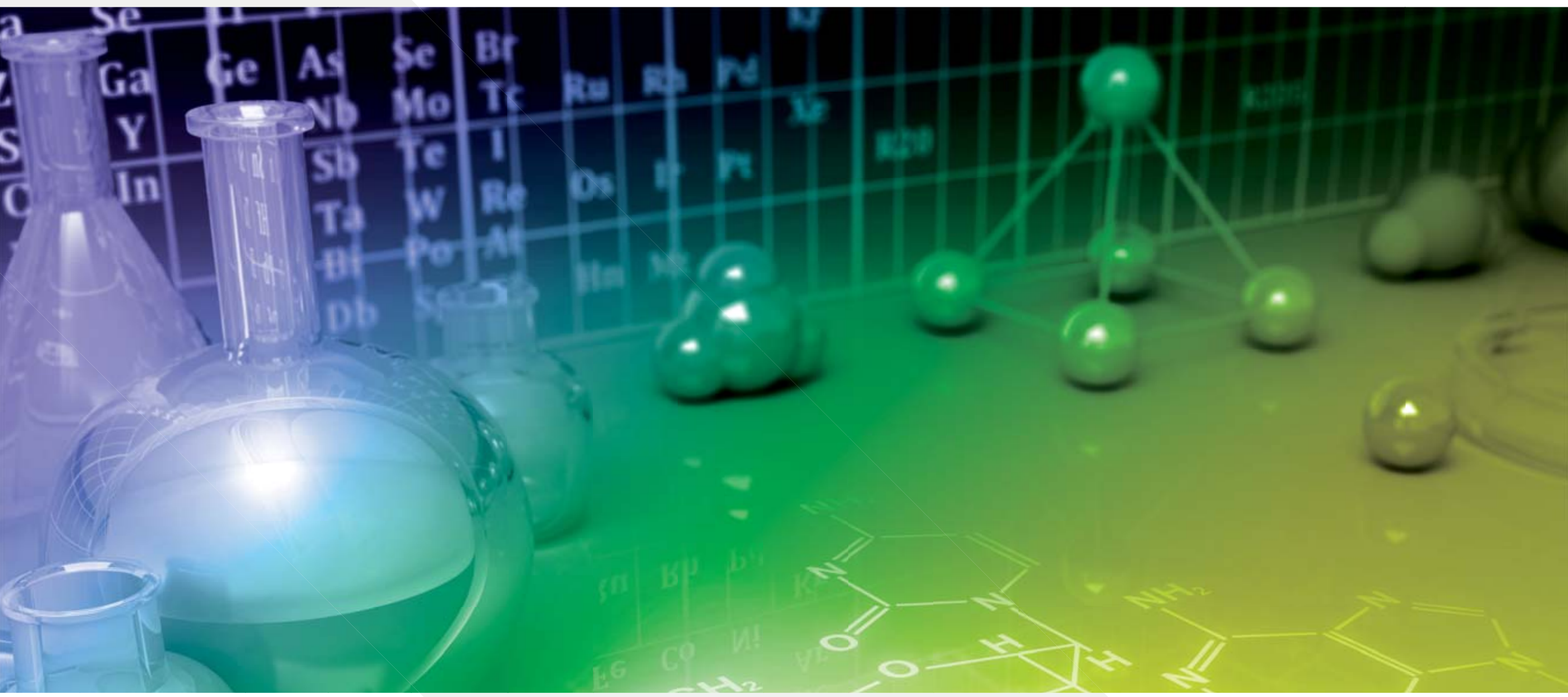
# CHEMICAL ENGINEERING & MATERIALS SCIENCE



# RESEARCH HIGHLIGHTS

MICHIGAN STATE UNIVERSITY | COLLEGE OF ENGINEERING

# department highlights

ENERGY & SUSTAINABILITY ▪ NANOTECHNOLOGY & MATERIALS ▪ BIOTECHNOLOGY & BIOMEDICAL ENGINEERING

The Department of Chemical Engineering and Materials Science at Michigan State University has vibrant research programs in both chemical engineering and materials science and engineering. The current faculty count stands at 29, including four University Distinguished Professors. Faculty members have received numerous awards and honors, including:

- the NSF CAREER Award
- the University Distinguished Faculty Award
- the Withrow Teaching Excellence Award
- and the Withrow Research Scholar Award.

Also included among the faculty ranks are multiple society Fellows (of the American Institute of Chemical Engineers, the American Institute of Chemists, the Society of Plastics Engineers, ASTM International, the American Ceramic Society, ASM International, ABET, and the American Physical Society).

Among the Department's achievements are:

- Total research expenditures of about $9,000,000
- Approximately 135 refereed publications and 9 patents per year
- Growth of the total undergraduate student population to 704
- Current graduate enrollments of 86 PhD students and 15 Master's students
- Several major research centers, including the Composite Materials and Structures Center, the Center for Revolutionary Materials for Solid State Energy Conversion (Department of Energy), and the Great Lakes Bioenergy Research Center (Department of Energy).

The mission of the MSU ChEMS Department is to be nationally recognized for excellence in research, teaching, and service. In support of this mission, four goals have been targeted:

- Provide leadership and excellence in conducting nationally recognized, innovative, and cutting-edge research
- Recruit high-performing students and deliver modern, high-quality graduate and undergraduate programs that produce top-notch graduates serving the needs of industry, government, and academia
- Offer outstanding professional and outreach services
- Conduct fundraising from the private sector, state, and federal sources, and provide stewardship in support of research, instruction, and service

As we look to the next decade, the Department has established strategic initiatives to ensure our continued ascension in productivity and prominence:

- Addition of new faculty to complement and supplement our research priorities
- Recruitment of a higher number and quality of PhD students
- Increase in the number of highly qualified undergraduate students and bachelor's degree graduates prepared to solve the problems of both today and tomorrow
- Enhanced support of endowments for fellowships, scholarships, professorships, and the discretionary excellence fund.

The department has positioned itself and established its research priorities to address critical 21st-century challenges such as energy and sustainability, nanotechnology and materials, and biotechnology and biomedical engineering.

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# from the chair

Reflecting on the 2014–15 academic year, I am excited by the continued growth of our department and the outstanding accomplishments of our faculty and students.

With more than 25 years of research excellence in the field of composite materials, MSU was tapped by President Barack Obama in January to be a core partner in the Institute for Advanced Composites Manufacturing Innovation (IACMI), a 122-member consortium funded by a more than $70 million commitment over five years from the U.S. Department of Energy. Under the direction of University Distinguished Professor Lawrence Drzal, MSU will lead the light-and-heavy-duty vehicle component of the IACMI.

## OUTSTANDING FACULTY

In the past year, numerous faculty members have distinguished themselves through prestigious awards and honors. University Distinguished Professor Bruce Dale was once again the top-ranked academic (ranked 14th) on *Biofuels Digest*'s list of the "Top 100 People in the Bioeconomy." Richard Lunt, assistant professor of chemical engineering and materials science, was awarded the Camille and Henry Dreyfus Award in Environmental Chemistry. Dr. Lunt also received the 2015 MSU Undergraduate Research Faculty Mentor of the Year Award, and was recognized in April by the MSU Innovation Center with an Innovation of the Year Award for his development of Transparent Photovoltaics. Christina Chan, the George W. Bissell Professor in Chemical Engineering and Materials Science, was among 10 MSU faculty members named as 2014 Beal Outstanding Faculty (formerly Distinguished Faculty), and Thomas Bieler, professor of chemical engineering, was awarded the department's 2015 Withrow Teaching Excellence Award.

Among CHEMS faculty members named to prestigious professional societies this year were Daina Briedis, who was named a 2015 Fellow of ASEE; and five CHEMS faculty members—Bruce Dale, Lawrence Drzal, Dennis Miller, Ramani Narayan, and R. Mark Worden—who were among the inaugural members of the MSU Chapter of the National Academy of Inventors.

## HIGH-ACHIEVING STUDENTS

Rebecca Carlson, a sophomore majoring in chemical engineering and Chinese, was awarded a prestigious Goldwater Scholarship. She became the second CHEMS student and third member of the College of Engineering to be named a national Goldwater Scholar in the past two years. Markus Downey, a PhD student in chemical engineering, was one of three students recognized during the Society of Plastics Engineers Automotive Composites Conference. Two materials science and engineering seniors—Thomas Heuser and John Suddard-Bangsund—were among 19 MSU students awarded National Science Foundation Research Fellowships in 2015. Heuser and Suddard-Bangsund were also recognized with MSU Board of Trustees awards for graduating with a perfect 4.0 GPA this spring. Maytham Alzayer (chemical engineering) was honored in April 2014 for her 4.0 GPA, as well.

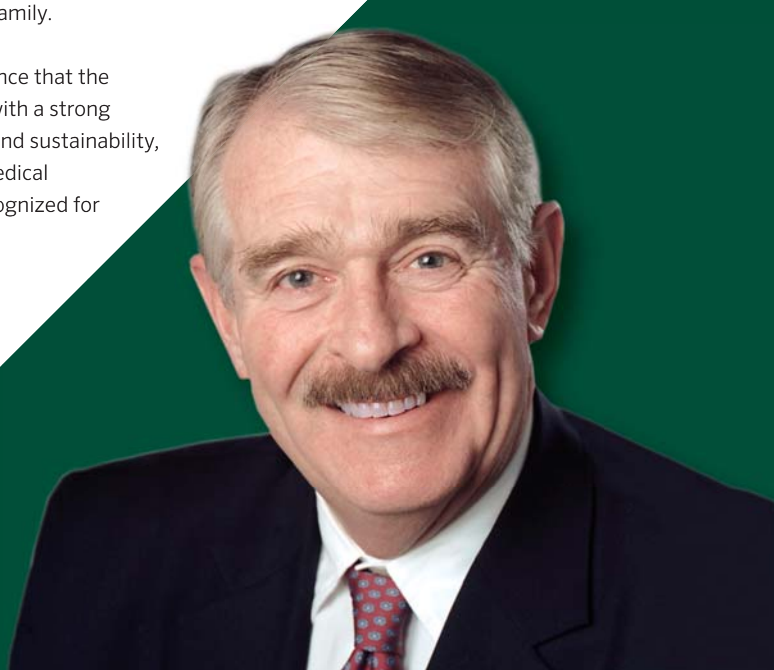
## DISTINGUISHED ALUMNI

On May 9, 2015, the Red Cedar Award, recognizing an outstanding ChEMS alumnus, was awarded to Craig A. Rogerson, president, chief executive officer, and chairman of the board of Chemtura Corporation.

The department will greatly benefit from a generous $2.5 million gift from alumnus Dave Lamp and his wife, Denise, to support scholarships and research—$2 million will establish the David L. and Denise M. Lamp Endowed Chair in Chemical Engineering, and the remaining $500,000 will enhance a scholarship fund previously created by the Lamp family.

I look upon these achievements with pride and great confidence that the superior efforts of our faculty, staff, and students, together with a strong research portfolio focused in three thematic areas—energy and sustainability, nanotechnology and materials, and biotechnology and biomedical engineering—will drive us in our mission to be nationally recognized for excellence in research, teaching, and service.

MARTIN C. HAWLEY
*Chairperson and Professor*



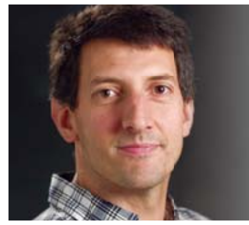
# FACULTY

## Kris Berglund

Kris Berglund is an MSU University Distinguished Professor of Food Science and Chemical Engineering. He obtained his PhD from Iowa State University in 1981 and Master's degree from Colorado State University in 1980. His research is on new and alternative uses of agricultural and forest raw materials; and separation, purification, and crystallization processes for food, pharmaceutical, and chemical industries. He is also focused on distilled beverage technology. He founded and has run the school's Artisan Distilling Program, since 1996. Recently, with his efforts, a beverage specialization was made available to MSU students in the fall of 2013.

## Thomas Bieler

Professor Thomas R. Bieler earned a B.A. in Applied Mechanics at University of California at San Diego in 1978 followed by a M.S. in Ceramic Engineering at University of Washington (Seattle) in 1980. He worked for five years at Sandia National Laboratory in Livermore on high-rate deformation. He completed his PhD in materials science (with a minor in continuum mechanics) at University of California–Davis in 1989, and has been at Michigan State University thereafter. His research focuses on characterization of mesoscale deformation mechanisms and plasticity modeling in titanium-based alloys, tin in the context of lead-free solder joints, and high-purity niobium used in superconducting particle accelerator cavities. With colleagues, he has published 270 papers, 34 of which have been cited more than 34 times. He was awarded the Distinguished Scientist/ Engineer and the Service Award in the Materials Processing and Manufacturing Division of the Mining, Metallurgical and Materials Society (TMS) in 2013.



## Carl Boehlert

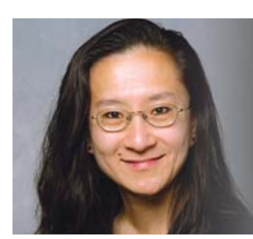
Carl Boehlert's research group is concentrating on understanding the deformation behavior of hexagonal close-packed metals, in particular, titanium and magnesium alloys, under extreme environments. The environments include a combination of both elevated temperatures and irradiation, and a variety of loading conditions are being used to mimic component use in commercial applications. *In situ* testing methods have been developed which allow for characterizing the surface deformation behavior during deformation in order to understand the deformation evolution. The work is being sponsored by the National Science Foundation and the Department of Energy.

## Daina Briedis

Daina Briedis is a both a faculty member in the Department of Chemical Engineering and Materials Science and Assistant Dean for Student Advancement and Program Assessment in the College of Engineering. Dr. Briedis has been involved in several areas of discipline-based education research (DBER) including student retention, curriculum redesign, and the use of technology in the classroom. Dr. Briedis helps facilitate student success through evidence-based improvement processes both at the college and the program level. She has been a co-PI on two NSF grants in the areas of integration of computation in engineering curricula and in developing comprehensive strategies to retain early engineering students. She also serves as Adjunct Director of Professional Development at ABET, Inc. She is active nationally and internationally in engineering accreditation and is a Fellow of ABET, the AIChE, and ASEE.

## Scott Calabrese Barton

Electrochemistry dramatically impacts numerous technologies for energy and chemical production, including modern electric and hybrid vehicles. A key enabler of these technologies are electrocatalysts. Dr. Barton's research group studies new electrocatalysts, materials, and electrode design for fuel cells and chemical conversion. Transition metal electrocatalysts are being studied as replacements for high-cost platinum, and could potentially lower the cost of fuel cell systems and enable practical fuel cell vehicles. Bioconversion involving enzyme electrocatalysts may lead to conversion of renewable resources to value-added chemicals. Professor Barton's group is developing electrodes to achieve such bioconversion, including catalysts for regeneration of enzyme cofactors, and high-surface carbon materials for immobilization of enzymes, catalysts, and cofactors. Throughout this work, mathematical models are incorporated to build understanding of electrochemical kinetics and transport, leading to tools for analysis and optimization of novel electrode architectures. He received his PhD in Chemical Engineering from Columbia University in 1999, after studying aerospace engineering at Notre Dame and MIT. He is the recipient of a prestigious CAREER award from the National Science Foundation and a Petroleum Research Fund award from the American Chemical Society.



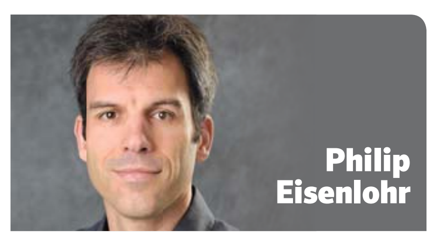
## Christina Chan

Many diseases do not have a proven means of prevention or effective treatments. Despite substantial advances in the development of drugs and therapies for treating complex, multi-factorial diseases such as cancer and Alzheimer's disease, current treatments assume one-size-fits-all and have been successful for some but not all cases of a given disease. Precision medicine is an emerging approach for treating complex diseases by taking into account the variability in genes and environment of each individual. The Chan laboratory takes a systems approach to understanding how molecular and environmental events influence one another as parts of an overall system, and together provides information that can improve the precision with which patients are categorized and treated.


Professor Martin A. Crimp joined Michigan State University in 1989, and focuses his research on the development and application of advanced electron microscopy techniques. He earned his BS and MS degrees in metallurgical engineering from Michigan Technological University and his PhD in materials engineering from Case Western Reserve University. Before joining MSU, he carried out two years of postdoctoral research at Oxford University. He has applied his expertise to the study of a wide range of materials classes including structural metals, magnetic multilayers, carbon and GaN nanowires and structures, self-assembled rare-earth nanostructures, and ceramic joining. He has been at the forefront of developing crystallographically based imaging techniques in scanning electron microscopy, bringing TEM based imaging approaches to the analysis of bulk structures using SEM. Additionally, he is an expert in failure analysis and brings these skills to the teaching of the MSE capstone design course. He has received an NSF Young Investigator award, the MSU Withrow Distinguished Researcher award, and the MSU Teacher Scholar award.


Professor Bruce E. Dale received his bachelors (summa cum laude) and masters degrees in chemical engineering from the University of Arizona in Tucson and the doctorate from Purdue University in 1979 under the direction of Dr. George T. Tsao, one of the early pioneers in biochemical engineering. Dr. Dale is currently University Distinguished Professor of Chemical Engineering at Michigan State University, also serving as editor in chief and founding editor of *Biofuels, Bioproducts and Biorefining*. He won the Charles D. Scott Award (1996) for contributions to the use of biotechnology to produce fuels and chemicals and the Sterling Hendricks Award (2007) for contributions to agriculture. He was named a Fellow of the American Institute of Chemical Engineers in 2011 and received the Award of Excellence of the Fuel Ethanol Workshop (also 2011). At number 14, he is the highest-ranked academic in the Top 100 People in Bioenergy (*Bioenergy Digest*), and has published over 250 journal papers and hold 42 US and international patents. Research interests include biofuels, the relationship between energy and societal wealth, life cycle assessment, and the design of integrated agroecosystems for producing sustainable fuels, chemicals, food, and animal feed.


Professor Lawrence T. Drzal is a University Distinguished Professor and Director of the Composite Materials and Structures Center. He conducts research on the synthesis, functionalization, processing, and manufacturing of carbon and glass fiber reinforced composite materials and graphene, nano-cellulose, and boron nitride nanomaterials. His current foci are on the combination of nanomaterials with fiber reinforced composites to produce multifunctional composite materials and the investigation into the use of inexpensive graphene nanoplatelets for various applications. Research from Drzal's group has led to a commercially viable method for manufacturing graphene nanoplatelets which have multiple desirable intrinsic properties that make them particularly attractive as additives to polymers and composites as well as for energy storage applications. Full advantage of these multifunctional nanomaterials requires not only a high level of dispersion but also novel processing methods to generate 2-D and 3-D microstructures within the polymers in which they are dispersed. Professor Drzal's group is investigating chemical, electrical, and flow methods to induce desirable structure of nanomaterials by themselves as well as within polymers to optimize their performance in structural and energy generation and storage applications. Professor Drzal and his students have published over 350 journal articles, been granted 35 patents, and spun off a company (XG Sciences) to manufacture graphene nanoplatelets. Professor Drzal has received numerous awards for his research and has been elected a Fellow in six national professional societies.




Associate Professor Philip Eisenlohr studied materials science and engineering at Universität Erlangen–Nürnberg, Germany, and received his PhD in 2004. Dr. Einsenlohr was research group leader at the Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany, before joining the Michigan State University Chemical Engineering and Materials Science department in 2013. His research focus is on mechanics of micro/nano-structured materials with an interest in basic science of plastic deformation mechanism in metals combined with the advancement of associated simulation methodologies. His major research target is the acceleration of materials design through Integrated Computational Materials

# FACULTY

Engineering (ICME) based on physically accurate descriptions of governing mechanisms. Investigated material classes include high-strength (twinning-induced plasticity) steels, titanium alloys, and tin-based solders.

## Martin Hawley

Martin C. Hawley, chairperson of the ChEMS Department, just celebrated 50 years as a Michigan State University faculty member. He received his BS and PhD in chemical engineering from MSU in 1961 and 1964, respectively. In 2001, he was named the first chairperson of the newly created Department of Chemical Engineering and Materials Science. Professor Hawley has taught the capstone design course for more than 40 years, with the designs from this course leading to the Department's award-winning tradition in the AIChE competition. He has broad research interests, including Carbon nanotube synthesis; chemical kinetics; reactor design; transport phenomena; enzyme kinetics; plasma reactions; electromagnetic processing of materials; petro-chemical processes; and biomass conversion processes.

## David Hodge

David Hodge obtained his undergraduate degree in chemical engineering from Auburn University with a specialization in pulp and paper engineering and obtained MS and PhD degrees in chemical engineering from Colorado State University. This was followed by work at the U.S. Department of Energy's National Renewable Energy Laboratory as post-doctoral researcher and a subsequent research faculty position at Luleå University of Technology in Sweden. In 2009 Dr. Hodge began a position as an assistant professor at Michigan State University in the Department of Chemical Engineering and Materials Science with a joint appointment in Biosystems & Agricultural Engineering. The research performed by Dr. Hodge's group at MSU addresses the challenges associated with the conversion and fractionation of plant cell wall biopolymers as well as food crops to renewable energy and fuels.

## Krishnamurthy Jayaraman

Dr. Jayaraman's research interests and expertise are processing, rheology, and microstructure development in polymer materials. These include composites, polymer nanocomposites, foams and porous composite products, thermoplastic olefin blends, elastomers, thermoplastic foams and thermoplastic vulcanizate blends (TPV). Current research projects include nonlinear rheology of polyamide based TPVs for extrusion and film blowing, die-drawing of porous polymer membranes for battery separators, texture development in die-drawn expanded polypropylene-talc composites, high-performance additives with nanoparticles for masking film in paint ovens,and modeling of expanding foam flow due to reaction in heated mold cavities with distributed vents.

## Wei Lai

Dr. Wei Lai is currently an assistant professor in the department of Chemical Engineering and Materials Science at Michigan State University. He received his B.S. and M.S. in Materials Science at the University of Science and Technology of China in 1998 and 2001. He obtained his PhD in Materials Science at the California Institute of Technology in 2007. Before joining MSU, he was a postdoctoral associate in the Department of Materials Science and Engineering at the Massachusetts Institute of Technology. His research interests are focused on the advanced materials and electroanalytical methods for energy storage and conversion applications.

## Andre Lee

Associate Professor Andre Lee obtained his Master's degree in Physics, and his Ph.D in Physics/Materials Science from University of Illinois, Urbana. He joined MSU in 1991. His research interests include viscoelastic and time-dependent properties of polymers and polymeric glasses, structure-property relationships of inorganic-organic hybrid polymers and nanocomposites, processing of hybrid nano-reinforced polymer, and nanostructured materials.

## Ilsoon Lee

Dr. Ilsoon Lee, associate professor in the Department of Chemical Engineering and Materials Science at Michigan State University, obtained his PhD in Chemical Engineering from University of Delaware in 2000. After a postdoc at MIT, he joined MSU in 2002. His 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.


Carl T. Lira is Associate Professor in the Department of Chemical Engineering and Materials Science at Michigan State University. He teaches thermodynamics at all levels, chemical kinetics, and material and energy balances. His research accomplishments include experimental measurements and modeling for liquid metals, supercritical fluids, adsorptive separations, and liquid-vapor, solid-liquid, and liquid-liquid phase equilibria. Professor Lira specializes in the study of thermodynamic properties of bio-derived fuels and chemicals via experiments and molecular simulations, and he collaborates in the MSU Reactive Distillation Facility. He has been recognized with the Amoco Excellence in Teaching Award, and multiple presentations of the MSU Withrow Teaching Excellence Award. He holds a B.S. from Kansas State University, and an M.S. and PhD from the University of Illinois, Champaign-Urbana, all in chemical engineering. He is co-author of the market leading textbook Introductory Chemical Engineering Thermodynamics, and he is involved in educational research using lexical analysis to interpret student misconceptions in thermodynamics.


Richard R. Lunt is an assistant professor at Michigan State University where his group focuses on understanding and exploiting excitonic photophysics and molecular crystal growth to develop unique thin-film optoelectronic devices. He earned his B.ChE. with Honors and Distinction from the University of Delaware in 2004 and his PhD in Chemical Engineering from Princeton University in 2010. He then worked as a post-doctoral researcher at MIT for a year before starting at MSU in 2011. His work has been featured in *Nature, NY Times*, Huffington Post, CNN, CBS, and NBC News, among others, and his innovative research has earned him a number of prestigious awards including the NSF CAREER Award, the Camille and Henry Dreyfus Mentor Award in Environmental Chemistry, the DuPont Young Investigator Award, and the GPEC Solar Innovation Award. He is the inventor of over 15 patents, the majority of which have been licensed, and recently won the Innovation of Year Award at MSU. He is also a founder of Ubiquitous Energy Inc., which is commercializing a range of seamless light-harvesting technologies.


Research in Dennis Miller's group focuses on the development of chemical pathways, catalysts, and processes to produce chemicals and biofuels from renewable biomass resources. Research projects involve both the development of new catalysts and reactor designs to carry out conversion of feed stocks to desired products, and the separation and purification of products from the reaction mixtures. Major efforts in current work are in reactive separations, where the chemical reaction and purification take place in a single process unit, and in upgrading low-cost intermediates from biomass such as ethanol and furan-based compounds to higher-profit products. Twenty U.S. patents along with numerous publications have come out of this work, and several technologies have been licensed for commercial development.


Donald Morelli is currently Professor of Materials Science at MSU and Director of the MSU/DOE Energy Frontier Research Center on Revolutionary Materials for Solid State Energy Conversion (RMSSEC). Prior to joining MSU in 2007, he spent 21 years in industry, first at General Motors Research Laboratories as a Senior Research Scientist, before moving to Delphi Corporation Research Labs in 1999, where he was staff research scientist and group leader of the nanomaterials group. Dr. Morelli received two GM Campbell Awards (1992 and 1997) for fundamental scientific research, the International Thermal Conductivity Conferences Fellowship Award (1993), and the Delphi Scientific Excellence Award (2004). He has been elected Fellow of the American Physical Society (2005) and was inducted into the Delphi Corporation Innovation Hall of Fame (2006). He currently serves as president of the International Thermoelectric Society. He has published over 150 scientific papers, coauthored four book chapters, and received 23 U.S. patents. His research has spanned a variety of topics, including: semimetals, conducting polymers, high-temperature superconductors, wide- and narrow-band gap semiconductors, high thermal conductivity crystals, thermoelectric materials, and magnetism. Dr. Morelli's research group at MSU continues to emphasize new semiconductors for thermoelectric energy conversion, as well as materials for thermal management. Dr. Morelli holds BS and PhD degrees in physics from the University of Michigan.


The Biobased Materials Research Group led by Ramani Narayan engineers new biobased and biodegradable-compostable polymer materials and bio processes using agricultural crops and residues (soybean and corn), lignocellulosic biomass, and algae. These products find commercial application in plastic bags, injection molded articles, thermoformed products, protective and insulation packaging, arts and crafts materials, and biomedical applications. 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); 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 Zeeland biobased products (www.zfsinc.com); and licensing four patents on thermoplastic modified starch and its copolymers with biopolyesters to Ingredion, Inc.


Jason D. Nicholas is an assistant professor in the Chemical Engineering and Materials Science Department at MSU. His group is focused on understanding and exploiting ionic conduction, ionic surface exchange, mechano-electro-chemical coupling, cost-effective processing methodologies, and hierarchy tailored microstructures to improve the performance of fuel cells, batteries, sensors, and other electro-chemically active devices. He earned a B.S. in Geoscience, with Honors, from Franklin & Marshall College in 2000, a M.S. in Materials Science and Engineering from the University of Illinois, Urbana-Champaign in 2003, and a PhD in Materials Science and Engineering from the University of California–Berkeley in 2007. After a postdoc position at Northwestern University, he joined the faculty at MSU in 2010. His innovative teaching and research have earned him a MSU Withrow Teaching Award and a National Science Foundation (NSF) Career Award. Jason has also taken several leadership roles, serving as the lead organizer for a NSF-sponsored "Solid Oxide Fuel Cells: Promise, Progress, and Priorities" workshop, the sole organizer for an annual Michigan State Girl Scout Science, Technology, Engineering, and Math (STEM) Demo Day, and a guest editor for a Journal of the Electrochemical Society Focus Issue on mechano-electro-chemical coupling. Updates on his work can be found at https://www.egr.msu.edu/nicholasgroup/.

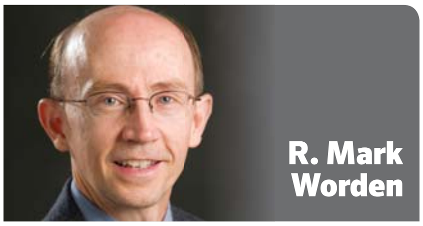

Robert Ofoli's research addresses the need for sustainable production of energy and materials. His primary interest is in the synthesis, characterization, assessment, and optimization of nanoscale catalysts and complexes that efficiently achieve the required transformations. Professor Ofoli's team focuses on four technological goals: reaction specificity; high reactivity under moderate reaction conditions; catalyst robustness and recyclability; and development of generic protocols to enable easy adaptation to other feedstock and products. Their general approach is to integrate rational catalyst design and synthesis, characterization and assessment, and modeling and simulation to understand structure-function relationships. Professor Ofoli is currently focusing on two areas of significant scientific and societal interest: biomimetic water oxidation to produce hydrogen and organic materials, and transformation of renewable materials to high-density liquid fuels capable of replacing those traditionally obtained from crude oil.


Turbulent flows occur ubiquitously with numerous examples in engineering, atmospheric science, oceanography, astrophysics, biology, and environmental science. Charles Petty is currently developing improved models for turbulence that will have a direct impact on the current use of advanced computational fluid dynamic methods for process design, process diagnostics, and process safety assessments by engineers and others. The results will support the discovery of new flow phenomena in disciplines that depend on accurate predictions of the mean velocity field and the mean pressure field. The goal is to develop a new class of low-order turbulent closure models that account for the transport of momentum, energy, and chemical constituents within single phase (and multiphase) rotating and non-rotating turbulent flows.


Dr. Yue Qi is an associate professor in the Chemical Engineering and Materials Science Department at MSU. She received her PhD in Materials Science from California Institute of Technology in 2001. She was a co-recipient of 1999 Feynman Prize in Nanotechnology for Theoretical Work during her PhD study. After her PhD, she spent 12 years working at Chemical Sciences and Materials Systems Lab, General Motors R&D Center, Warren, MI. At GM, she led multi-scale modeling research to solve problems related to forming and machining of lightweight alloys, and developing energy materials for batteries and fuel cells. She won three GM Campbell awards for outstanding research on various topics and TMS Young Leader Professional Development Award. Her recent research interest is integrating material failure model with battery life prediction. She has published more than 80 peer-reviewed journal papers with more than 2,000 citations.


One achievable goal of the 21st century is "personalized medicine," the design of diagnostics and therapeutics specifically for a single patient. The Applied Biomolecular Engineering Laboratory (ABEL), led by S. Patrick Walton, is currently working on development of both novel therapeutics and diagnostics, specifically on technologies that rely on nucleic acids (i.e., DNA and RNA). Areas of investigation include designing nucleic acid–based therapeutics based on understanding their mechanism of action, and developing diagnostics to measure protein levels in parallel. Recent foci have been a new class of therapeutics, short, interfering RNAs, with the goal of developing guidelines for designing these molecules. Additionally, Professor Walton is developing a technique for parallel measurements of transcription factors, proteins that help the cell respond to stimuli, using a solution-phase magnetic bead-based approach.


Engineering life is a broad-stated goal of the new generation of biological engineers. These engineers seek to design novel functions rather than rely on a catalog of "parts" culled from nature. For proteins, imparting novel and specific functions is a difficult problem because protein structures are only marginally stable, protein structure-function relationships are not well understood, and many targeted small molecule substrates differ by as little as a single hydroxyl group or a methyl bond. Tim Whitehead's group is working to solve the problem of engineering proteins. They use and develop computational techniques to design proteins for new functions, have pioneered experimental approaches to comprehensively assess the effect of a protein's sequence on its desired function, and have imparted evolutionary and computational ideas to formulate efficient routes to optimize protein function. Professor Whitehead is now interested in optimizing proteins for diverse applications like vaccine design and creating the next generation of biofuels.




R. Mark Worden's research group integrates engineering and biological principles to study two main research areas. The first area, biomimetic interfaces, involves understanding the mechanisms by which biological systems operate, and then applying those mechanisms in new ways. Professor Worden's lab is using artificial cell membranes to study nanoparticles toxicity. He is also studying protein "nanowires," produced by certain bacteria, that are believed to be conductive enough for use in new types of electronics and sensors. The second main research area, microbial catalysis, uses microorganisms to carry out desired chemical reactions. One example is gas fermentations, in which microorganisms convert energy-rich gases, such as hydrogen or methane, into high-value products. In collaboration with the nearby Michigan Biotechnology Institute, new types of microbubble-fed reactors are being developed for gas-based fermentations.

# FACULTY RESEARCH

# Kris Berglund

University Distinguished Professor | berglund@msu.edu | 517.974.3030 | 3815 Technology Blvd., Suite A114, Lansing, MI 48910


**RESEARCH INTERESTS**

Value-added products from agricultural and forest raw materials

**LAB LOCATION**

Michigan Biotechnology Institute, 3815 Technology Blvd., Suite A114, East Lansing MI

**GROUP MEMBERS**

Jacob Rochte, Nicole Shriner, George Cain

**RECENT PATENTS GRANTED** (18 TOTAL)

Berglund, K. A.; Rossman, P. K. Extraction of fusel alcohols from ethanol fermentation products. US patent 8981166, March 17, 2015.

Berglund, K. A; Rova, U.; Enman, J. Method for producing eritadenine in liquid phase fermentation. US patent 8053217, November 8, 2011.

**WEBSITE**

http://www.chems.msu.edu/people/profile/berglund

**CURRENT RESEARCH FOCUS**

Our group's activities are aimed at the creation of value-added products utilizing raw materials obtained from agricultural and forest raw materials. In particular, we utilize fermentation processes to develop integrated production for foods, beverages, biochemicals, and biofuels.

- ***Beverage technology.*** The artisan distilling industry in Michigan is poised to undergo significant expansion in the next few years resulting in positive economic impact for the state. Challenges for the entrepreneurs entering this business are access to technological expertise and facilities to develop and market products. An additional complication of the distilled spirits industry lies in the regulations governing it. Unlike beer and wine, there is no minimum amount of spirits that can be produced without Federal and State licenses. Furthermore, it is required to have constructed an operational distillery in order to apply for a Federal license. These regulations place the potential new producer in the position that in order to attract investment it is necessary to produce products and show their market value, but to do so, it is necessary to have the investment in a plant to get a license. We work to break this cycle by assisting new entrepreneurs in development and marketing of their spirits in order to attract the required investment for construction of their own facility.

- ***Upgrading forest byproducts.*** Xylose derived from hemicellulose is a low-cost source of substrate for butyric acid fermentation given that extraction could be integrated into current industrial pulp and paper processes yielding hemicellulosic sugars for the fermentation while retaining the properties of the cellulose fraction to be used in the subsequent pulp production. One of the main issues concerning such an integration is that hydrolysis of hardwood hemicellulose releases not only xylose but also acetic acid (up to 40 g/L), a microbial inhibitor. To achieve biologically conversion of xylose to butyric acid, the inhibiting acetic acid must either be removed from the extraction broth or the fermentation strain adapted to tolerate such high levels. This study focuses on the impact of high levels of acetic acid on *C. tyrobutyricum* fermentation growth kinetics and product yields in order to establish a process with extracted xylose as a substrate without requiring the removal of the toxic acetic acid from the broth.

**RECENT PUBLICATIONS**


Robert Nilsson; Fredric Bauer; Sennai Mesfun; Christian Hulteberg; Joakim Lundgren; Sune Wännström; Ulrika Rova; Kris A. Berglund. "Techno-economics of carbon preserving butanol production using a combined fermentative and catalytic approach," *Bioresource Technology*. 2014;161:263–269. (2014)

Adam M. Jaros; Ulrika Rova; Kris A. Berglund. "Acetate adaptation of clostridia tyrobutyricum for improved fermentation production of butyrate," *SpringerPlus*. 2013;2(1):1–8. (2013)

D. Graiver; R. Dacomba; M. Khawaji; A. Jaros; K. A. Berglund; R. Narayan. "Steel-corrosion inhibitors derived from soybean oil JAOCS," *Journal of the American Oil Chemists' Society*. 2012;89(10):1895–1903. (2012)

Josefine Enman; David Hodge; Kris A. Berglund; Ulrika Rova. "Growth promotive conditions for enhanced eritadenine production during submerged cultivation of *Lentinus edodes*," *Journal of Chemical Technology and Biotechnology*. 2012;87(7):903–907. (2012)

Adam Jaros; Ulrika Rova; Kris A. Berglund "Effect of acetate on fermentation production of butyrate," Cellulose Chemistry and Technology. 2012;46(5–6):341–347. (2012)

# Thomas Bieler

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**RESEARCH INTERESTS**

Grain boundaries, crystallographic texture, crystal plasticity, microstructure evolution, damage nucleation

**GROUPS**

Solder research group, niobium research group, titanium research group

**WEBSITE**

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**SPECIAL EQUIPMENT AVAILABLE**

Orientation imaging microscopy, *in situ* deformation stage in SEM

**GROUP MEMBERS**

Chen Zhang, Harsha Phukan, Yang Su, Bret Dunlap, Jason Zhou, Aboozar Mapar, Di Kang, Mingmin Wang, Mengge Zhao

**PATENTS GRANTED**

Bieler, T. R.; Subramanian, K.N.; Choi, S. Methods for producing lead-free in-situ composite solder alloys. US patent 7771547, August 10, 2010.

Bieler, T. R.; Yallapragada, V. R.; Wang, H.; Drzal, L.T. Apparatus for the preparation of metal matrix fiber composites. US patent 5891249, April 6, 1999.

**CURRENT RESEARCH FOCUS**

Orientation imaging microscopyTM (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 3-D 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. Three materials under investigation:

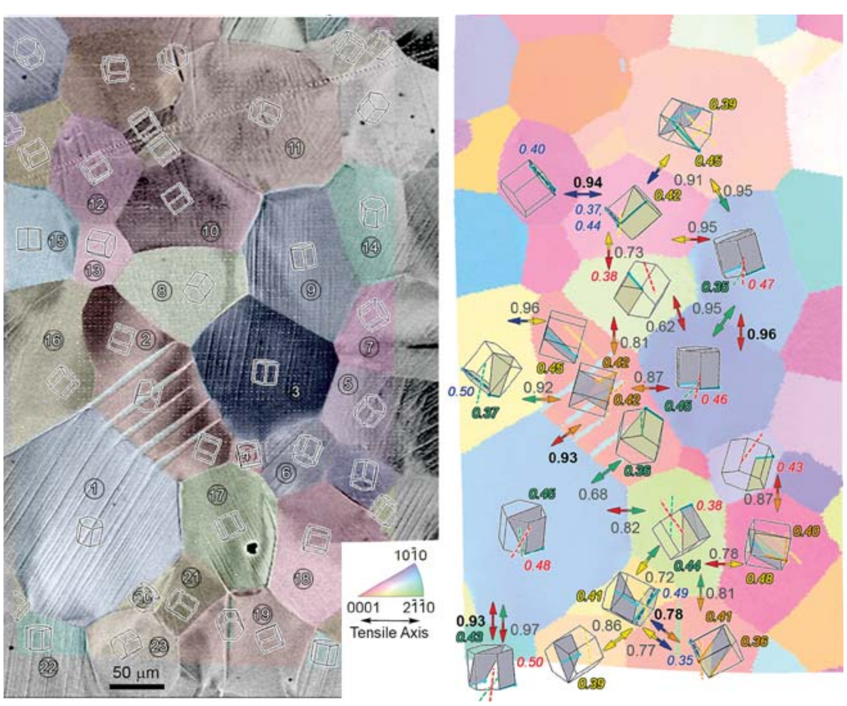


**FIGURE 1.** A microstructural patch illustrating heterogeneous deformation and slip activity in commercial purity titanium deformed in tension. Crystal orientations are illustrated, slip system traces and their Schmid factors are indicated in different colors, and slip transfer parameters computed. There is clear evidence for slip transfer in boundaries with high (bold black) values with prism (red) or basal (blue) slip.

- ***Damage nucleation in titanium and titanium alloys***, NSF/DFG Materials World Network Grant and DOE/BES SISGR Grant, with Martin A. Crimp, Carl J. Boehlert, Philip Eisenlohr at MSU, collaboration with Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany.

  Figure 1 shows a patch of equiaxed microstructure of a grade 1 pure titanium sample surface strained by bending to about 3% strain. The right side shows which slip systems could lead to slip transfer, which affects the 'transparency' of a grain boundary to slip. Slip planes are indicated geometrically within unit cells, and colored dashed lines show the slip plane traces observed on the surface (evident on left side). Slip transfer is most likely when active prism (red) or basal (blue) slip systems (colored numbers indicate Schmid factors, *m*) have a high degree of alignment indicated by bold black numbers with slip or twin systems in a neighboring grain, e.g., the boundary between grains 3 and 9 show prism slip transfer. Boundaries with gray slip transfer numbers describe either lower values (below 0.9) or alignment between slip systems involving less active slip systems on pyramidal planes (green and gold plane traces and Schmid factors). There are two instances of twin nucleation at grain boundaries (gold plane traces), one with strong evidence for slip transfer (0.93 between grains 1 and 2) and one less favored instance between grains 21 and 19 with low slip transfer (0.78).

  This same material is under investigation in samples deformed while monitoring grain strain using synchrotron x-ray diffraction in beamline 1ID-E at the Advanced Photon Source (APS). This method uses diffraction based tomography to identify stress states in grains throughout the volume of a tensile sample. About ⅓ of these analyzed twins have neighboring grains with active slip systems that could have triggered the observed twin similar to that observed in Figure 1 between grains 1 and 2.

- ***Microstructural evolution during thermo-mechanical cycling in lead-free solder joints***, NSF/GOALI with Cisco Systems, Inc., with Farhang Pourboghrat at MSU and Tae-kyu Lee at Cisco Systems, Inc.

  Figure 2 shows synchrotron characterization of an *in situ* tensile test of a multi-crystal Sn-3Ag-0.5Cu solder joint. Data were collected using a near-field detector that provides information about grain shapes—from which a 3-D model of each grain can be built from many 4 mm layers. The lower half of the figure shows data from far-field detectors, which provide information about stress and strain tensors at each dot, (which represent each grain or subgrain and its size). These data are new, and will be mined to identify how particular slip systems lead to low angle boundaries and internal stress states that influence which slip systems operate.

- ***Characterization and modeling of deformation and recrystallization in high purity Nb for particle accelerators***, DOE/OHEP, with F. Pourboghrat and N.T. Wright at MSU, and C. Compton at FRIB.

  High purity Nb is used for particle accelerator cavities (the structures that accelerate particles), but because of its limited use, the fundamental physics of deformation processing and microstructure evolution are not well understood. We are assessing details of slip deformation mechanisms to develop material models that can be used to optimize forming operations that lead to more consistent performance of cavities. We have examined how removal of dislocations with heat treatment changes which slip systems are activated during deformation, and this implies that prediction of deformation depends sensitively on prior heat treatments.

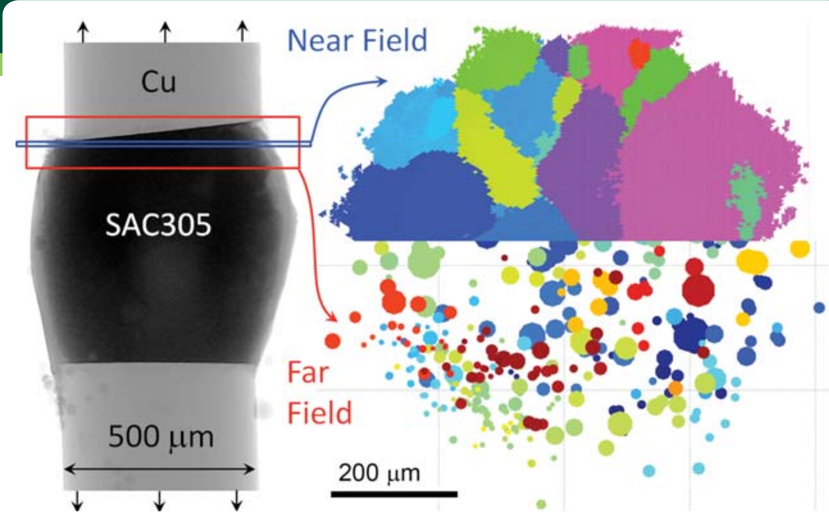


**FIGURE 2.** HEDM measurement of an *in situ* tensile experiment of a polycrystalline solder joint. Near field measurements provide orientation maps in multiple 4 mm slices, and colored dots in the far field measurements provide center of mass position, crystallite size, average stress tensor, and orientation within a 100 µm thick slice. Fewer grains were present in the middle of the joint than near the interfaces. Indexed using MIDAS software under development at Sector 1, APS.

## RECENT PUBLICATIONS

H. Li; C.J. Boehlert; T.R. Bieler; M.A. Crimp. "Examination of the distribution of the tensile deformation systems in tension and tension-creep of Ti-6Al-4V (wt.%) at 296 K and 728 K," *Philosophical Magazine.* (2015)

Bite Zhou; Quan Zhou; Thomas R. Bieler; Tae-kyu Lee. "Slip, Crystal Orientation, and Damage Evolution During Thermal Cycling in High-Strain Wafer-Level Chip-Scale Packages," *Journal of Electronic Materials.* 2015. (2015)

C. Zhang; H. Li; P. Eisenlohr; W. Liu; C.J. Boehlert; M.A. Crimp; T.R. Bieler. "Effect of realistic 3D microstructure in crystal plasticity finite element analysis of polycrystalline Ti-5Al-2.5Sn," *International Journal of Plasticity.* 2015;69:21–35. (2015)

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Tamin Tai; Behnood G. Ghamsari; Thomas R. Bieler; Teng Tan; X.X. Xi; Steven M. Anlage. "Near-field microwave magnetic nanoscopy of superconducting radio frequency cavity materials," *Applied Physics Letters.* 2014;104(23). (2014)

Payam Darbandi; Tae-Kyu Lee; Thomas R. Bieler; Farhang Pourboghrat. "Crystal plasticity finite element study of deformation behavior in commonly observed microstructures in lead free solder joints," *Computational Materials Science*. 2014;85:236–243. (2014)

Bite Zhou; Govindarajan Muralidharan; Kanth Kurumadalli; Chad M. Parish; Scott Leslie; Thomas R. Bieler. "Microstructure and sn crystal orientation evolution in Sn-3.5Ag lead-free solders in high-temperature packaging applications," *Journal of Electronic Materials.* 2014;43(1):57–68. (2014)

Thomas R. Bieler; Scott C. Sutton; Bret E. Dunlap; Zackery A. Keith; Philip Eisenlohr; Martin A. Crimp; Brad L. Boyce. "Grain boundary responses to heterogeneous deformation in tantalum polycrystals," *JOM.* 2014;66(1):121–128. (2014)

Subhasis Mukherjee; Abhijit Dasgupta; Bite Zhou; Thomas R. Bieler. "Multiscale modeling of the effect of micro-alloying Mn and Sb on the viscoplastic response of SAC105 solder," *Journal of Electronic Materials.* 2014;43(4):1119–1130. (2014)

David J. Schrock; Di Kang; Thomas R. Bieler; Patrick Kwon. "Phase dependent tool wear in turning Ti-6Al-4V using polycrystalline diamond and carbide inserts," *Journal of Manufacturing Science and Engineering, Transactions of the ASME.* 2014;136(4). (2014)

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Thomas R. Bieler; Leyun Wang; Armand J. Beaudoin; Peter Kenesei; Ulrich Lienert. "In situ characterization of twin nucleation in pure Ti using 3D-XRD," *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science.* 2014;45(1):109–122. (2014)

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# Carl Boehlert

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**RESEARCH INTERESTS**

Physical metallurgy

**LAB LOCATION**

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**WEBSITE**

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**SPECIAL EQUIPMENT AVAILABLE**

Creep testing machines, fatigue testing machine, tensile testing machine, metallography preparation equipment

**GROUP MEMBERS**

COLLABORATING FACULTY: Thomas Bieler, Martin Crimp, and Philip Eisenlohr. CURRENT PHD GRADUATE STUDENTS: Vahid Khademi, Ajith Chakkedath, Uchechi Okeke, Aida Amroussa, Xiaolu Yin. CURRENT VISITING SCHOLAR: Huan Wang.

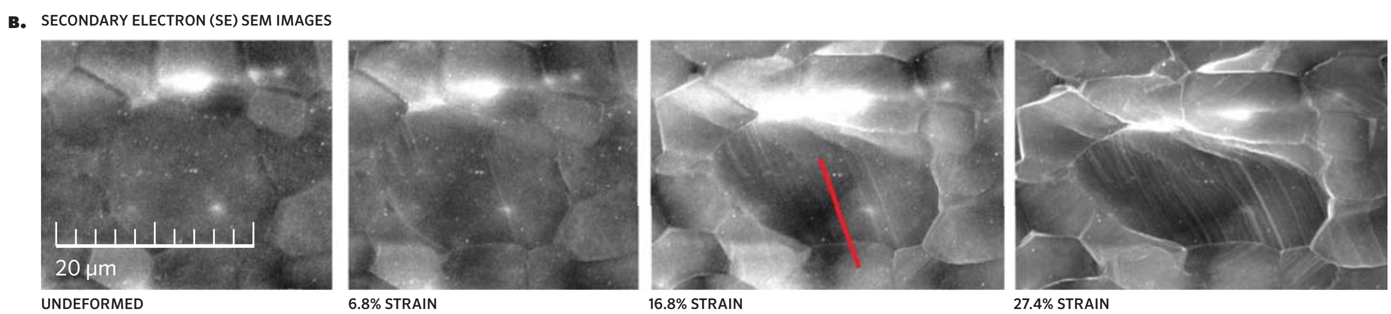
**PATENTS GRANTED**

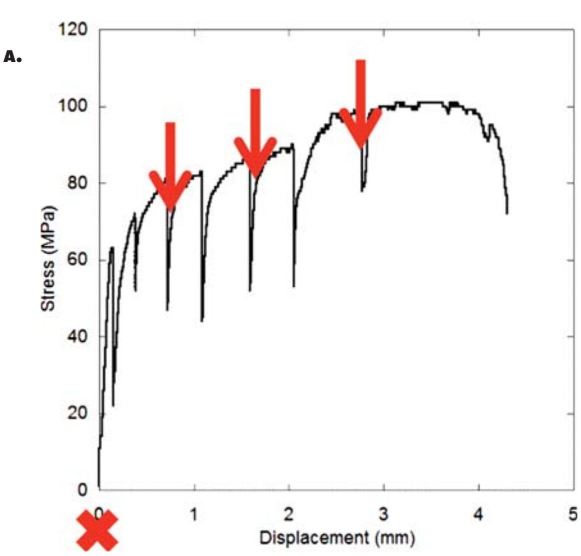
Boehlert, C.J. Ti, Al, and Nb Alloys for Biomedical Applications. US Patent 7,682,473, November 9, 2009.

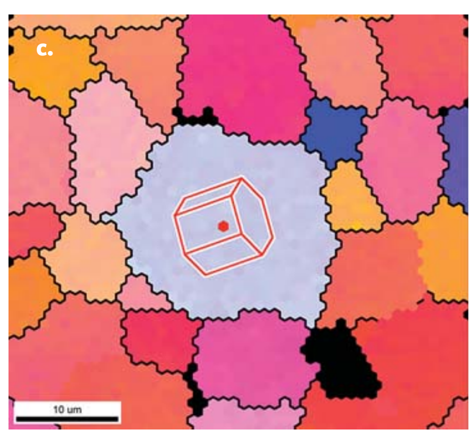
**CURRENT RESEARCH FOCUS**

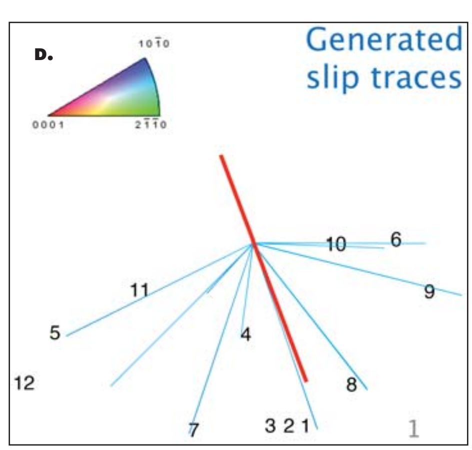
The research group of Associate Professor Carl Boehlert is concentrating on understanding the deformation behavior of hexagonal close packed metals, in particular titanium and magnesium alloys, under extreme environments. The environments include a combination of both elevated temperatures and irradiation, and a variety of loading conditions are being used to mimic component use in commercial applications. *In situ* testing methods have been developed which allow for characterizing the surface deformation behavior during deformation in order to understand the deformation evolution. The work is being sponsored by the National Science Foundation and the Department of Energy and the Michigan State University Strategic Partnerships Grant.

An extruded Mg-1Mn-1Nd(wt.%) (MN11) alloy was tested in




E.

| Schmid factor | Slip system | Plane/ direction |
|---|---|---|
| 0.44 | 3 | (0001) [-1-120] |
| 0.41 | 7 | (11-2-2) [-1-123] |
| 0.40 | 8 | (-12-12) [1-213] |
| 0.40 | 12 | (2-1-12) [-2113] |
| 0.22 | 2 | (0001) [-12-10] |
| 0.21 | 1 | (0001)[-2110] |
| 0.21 | 9 | (-2112) [2-1-13] |
| 0.20 | 11 | (1-212) [-12-13] |
| 0.11 | 5 | (10-10) [1-210] |
| 0.11 | 4 | (01-10) [2-1-10] |
| 0.02 | 10 | (-1-122) [11-23] |
| 0.00 | 6 | (-1100) [11-20] |

**FIGURE 1.** Example of the slip trace analysis performed for a tensile-tested MN11 sample. The images are (A) stress versus displacement curve, (B) scanning electron microscopy (SEM) images taken at different stresses and strains, (C) electron backscattered diffraction (EBSD) orientation map of the same area in the SEM images, (D) the slip system selection; note that slip system 3 was the selected system based on the match and this corresponds to the (0 0 0 1) plane and [-1 -1 2 0] direction. The Schmid factors for all the slip systems are tabulated in (E).

tension in a scanning electron microscope (SEM) at temperatures of 323K (50°C), 423K (150°C), and 523K (250°C) in order to analyze the local deformation mechanisms through *in situ* observations. Electron backscatter diffraction (EBSD) was performed before and after the deformation and a slip-trace analysis was performed to identify the distribution of the deformation mechanisms as a function of stress/strain, see Figure 1. It was found that the tensile strength decreased with increasing temperature, and the relative activity of different twinning and slip systems was quantified. At 323K (50°C), extension twinning, basal, prismatic <a>, and pyramidal <c+a> slip were active. Much less extension twinning was observed at 423K (150°C). At 523K (250°C), twinning was not observed, and basal slip controlled the deformation.

These *in situ* experiments provide new insight on the deformation mechanisms of Mg-RE alloys. The relative contributions of the different deformation modes as a function of temperature are illustrated in Figure 2. It appeared that the activity of basal and non-basal slip was more balanced at lower temperatures compared with higher temperatures, where basal slip was dominant. The percentage of basal slip increased from 50% to 75% to 87% with increasing temperature from 323K (50°C) to 423K (150°C) to 523K (250°C), respectively. Twinning decreased from 31% to 3% to 0% with increasing temperature from 323K (50°C) to 423K (150°C) to 523K (250°C), respectively. The prismatic slip and pyramidal <c+a> slip system percentages did not change markedly with temperature. Upon grouping the twin and basal slip systems, the percentage of these "soft" modes remains basically the same for all three of the deformation temperatures analyzed. Essentially, the strain accommodated by twins is replaced by basal slip at the higher temperatures. Overall, the results suggest that the activation of basal slip compared to non-basal slip and twinning is easier at higher temperatures compared with lower temperatures and the relative activity of twinning is reduced significantly with increasing temperature.

The following conclusions were drawn from this study:

The relative slip activity between the basal and prismatic and pyramidal slip systems was quantified. At 323K (50°C), extension twinning, basal, prismatic <a>, and pyramidal <c+a> slip were active. At 423K (150°C), much less extension twinning was observed. At 523K (250°C), twinning was not observed, and basal slip controlled the deformation.

Overall the prismatic slip and pyramidal <c+a> slip system percentages did not change markedly with temperature and the percentage of these basal slip+twinning modes remained basically the same for all three of the deformation temperatures. Therefore, the strain accommodated by twinning at the lower temperatures was replaced by basal slip at the higher temperatures.

The CRSS of basal slip is believed to decrease with increasing temperature for MN11.

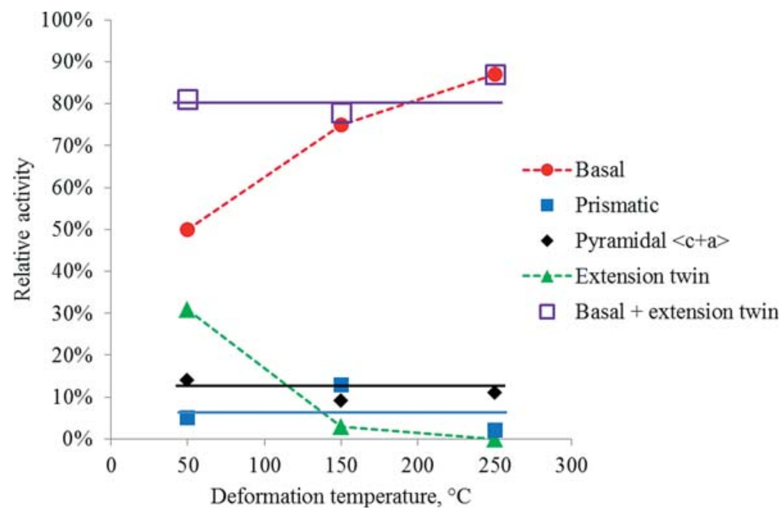



**FIGURE 2.** Plot depicting the percentages of each deformation mode with respect to temperature.

## RECENT PUBLICATIONS

H. Li; C.J. Boehlert; T.R. Bieler; M.A. Crimp. "Examination of the distribution of the tensile deformation systems in tension and tension-creep of Ti-6Al-4V (wt.%) at 296 K and 728 K," *Philosophical Magazine*. 2015. (2015)

Hongmei Li; Carl J. Boehlert; Thomas R. Bieler; Martin A. Crimp. "Analysis of the Deformation Behavior in Tension and Tension-Creep of Ti-3Al-2.5V (wt pct) at 296 K and 728 K (23°C and 455°C) Using In Situ SEM Experiments," *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*. 2014;45(13):6053–6066. (2014)

R. Muñoz-Moreno; E.M. Ruiz-Navas; C.J. Boehlert; J. Llorca; J.M. Torralba; M.T. Pérez-Prado. "Analysis of crystallographic slip and grain boundary sliding in a Ti-45Al-2Nb-2Mn (at%)-0.8vol%$TiB_2$ alloy by high temperature in situ mechanical testing," *Materials Science and Engineering A*. 2014;606:276–289. (2014)

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M.T. Pérez-Prado; J. Llorca; C.J. Boehlert. "Foreword: Processing-microstructure-property relationships & amp; deformation mechanisms of magnesium alloys," *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*. 2014;45(8):3195–3196. (2014)

Ajith Chakkedath; Jan Bohlen; Sangbong Yi; Dietmar Letzig; Zhe Chen; Carl J. Boehlert. "The effect of Nd on the tension and compression deformation behavior of extruded Mg-1Mn (wt pct) at temperatures between 298 K and 523 K (25°C and 250°C)," *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*. 2014;45(8):3254–3274. (2014)

H. Wang; Q.D. Wang; C.J. Boehlert; D.D. Yin; J. Yuan. "Tensile and compressive creep behavior of extruded Mg-10Gd-3Y-0.5Zr (wt.%) alloy," *Materials Characterization*. 2014;99:25–37. (2014)

# Scott Calabrese Barton

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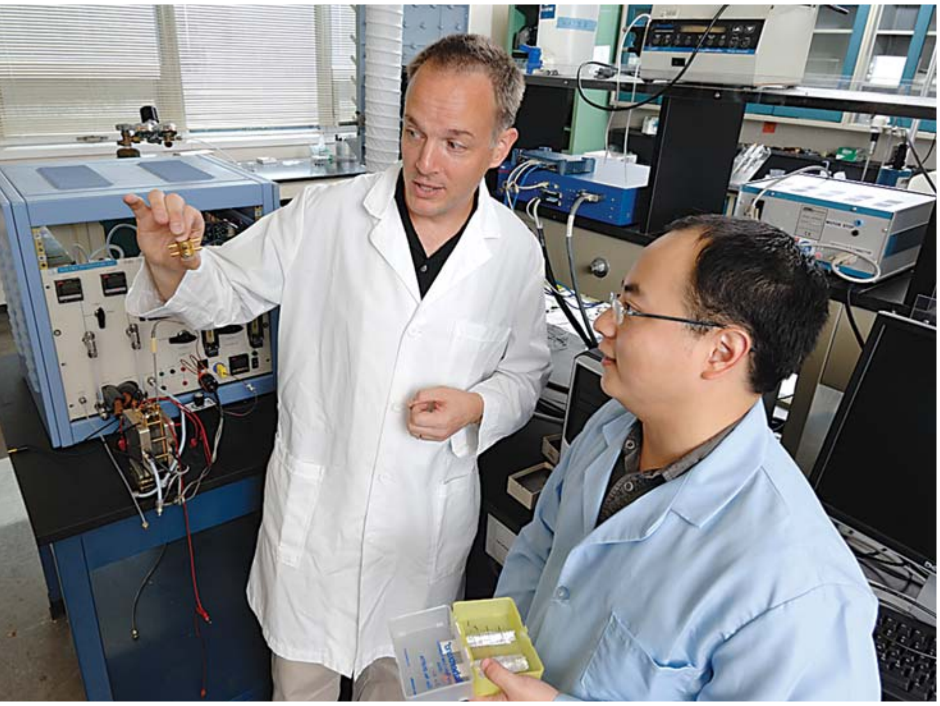

#### RESEARCH INTERESTS
Electrochemistry and electrocatalysis, from theory to experiment

#### LAB & LOCATION
Electrochemical Energy Lab, 428 S. Shaw Lane, Room 3250

#### WEBSITE
http://www.msu.edu/~scb

#### GROUP MEMBERS
Cenk Gumeci, Nate Leonard , Duyen Do, Yuanchao Liu, Erica Earl, Jacob Anibal, Nam Tran

#### PATENTS GRANTED
Banta, S.; Calabrese Barton, S. A.; Wheeldon, I.R. Self-assembling protein hydrogel with bio-active protein. US patent 8415290, April 9, 2013.

Heller, A.; Mano, N.; Kim, H.; Zhang, Y.; Mao, F.; Chen, T.; Calabrese Barton, S. A. Miniature biological fuel cell that is operational under physiological conditions, and associated devices and methods. US patent 7368190, May 6, 2008.

#### CURRENT RESEARCH FOCUS
Our research addresses engineering and materials issues in fuel cells, particularly mass transport within fuel cell electrodes. We focus on non-precious metal catalysts based on redox enzymes and transition metals, which have lower costs compared to precious metals, but are challenging in terms of overall activity and stability and often are implemented at high loadings that lead to transport limitations. Below are brief descriptions of current projects.

- ***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 1). Activity approaches that of precious-metal platinum in acid and alkaline electrolytes.

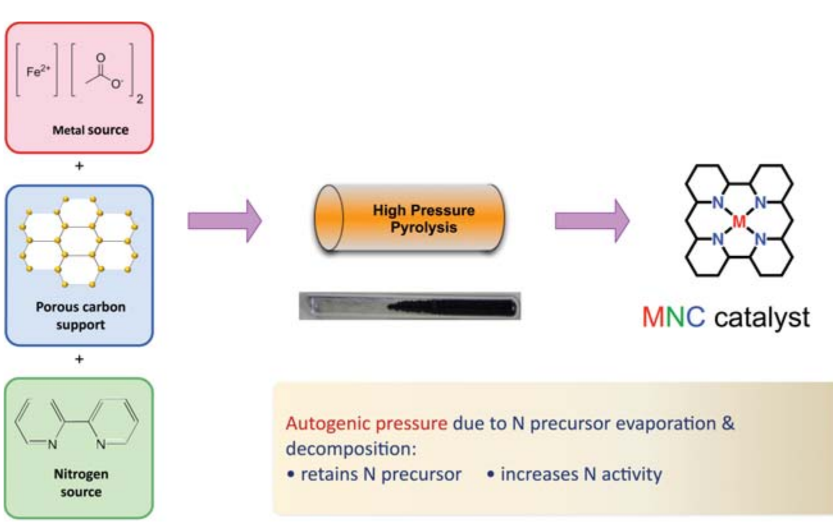


**FIGURE 1.** High-pressure pyrolysis process for non-precious metal catalyst production. Retention of volatile intermediates leads to increased nitrogen activity and site density.

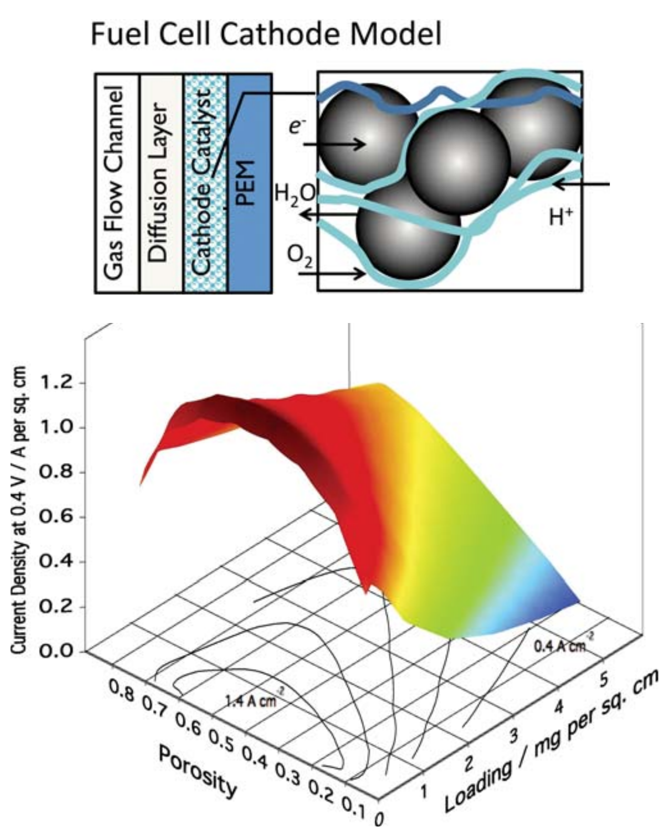


**FIGURE 2.** Cathode model schematic and optimization results. Maximum performance at low voltage (high current density) is achieved at low catalyst loading.

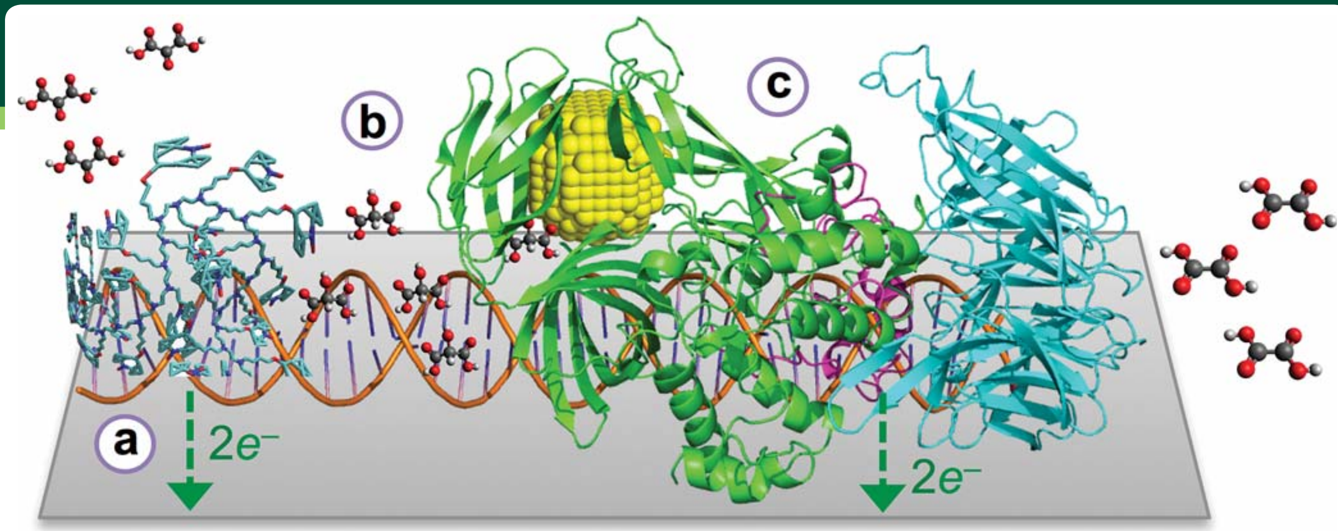


**FIGURE 3.** (A) Tartronic acid oxidation to mesoxalic acid at TEMPO catalyst; (B) facilitated transport of mesoxalic acid along DNA; (C) oxidation of mesoxalic acid to oxalic acid via catalysis by PtRu nanoparticle – AldDH adduct.

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 2).

SPONSOR: DOE. COLLABORATORS: Northeastern University, Pajarito Powders LLC, Nissan Technical Center NA, et al.

- ***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 3).

  SPONSOR: Army. COLLABORATORS: University of Utah, University of New Mexico, Columbia University, UC Riverside.

- ***Electrospun nanofibers for transition metal electrocatalalysis and bioelectrocatalysis.*** Introduction of non-precious electrocatalysts to electrochemical processes is plagued by poor transport properties owing to the large catalyst loading of relatively low-activity catalysts. We are to developing two classes of electrocatalysts based on electrospun carbon nanofibers. Electrospinning is a well-established, industrial-scale process producing carbon fibers with diameters ranging from 100 nm to over 1 micron and can be engineered with a range of structural, morphological, and surface properties for engineering and control of advanced porous electrodes (Figure 4). We implement these materials in two ways: (A) as precursor materials for preparation of metal-nitrogen-carbon (MNC) electrocatalysts for oxygen reduction, and (B) as support materials for preparation of enzymatic bioelectrodes. MNC electrocatalysts have applicability to low-temperature fuel cells for transportation and portable power. Bioelectrodes may be applied to biosensor, chemical conversion, and small-scale portable power environments.

  UNSPONSORED.

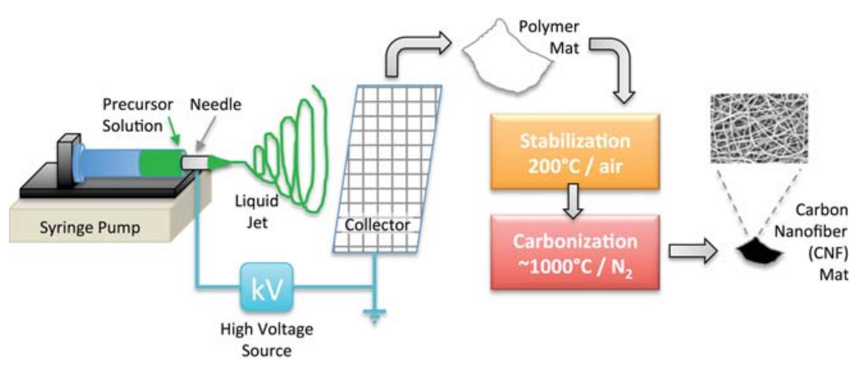


**FIGURE 4.** A basic experimental setup for electrospinning, followed by thermal treatment to produce carbon nanofiber (CNF) mats.

## RECENT PUBLICATIONS

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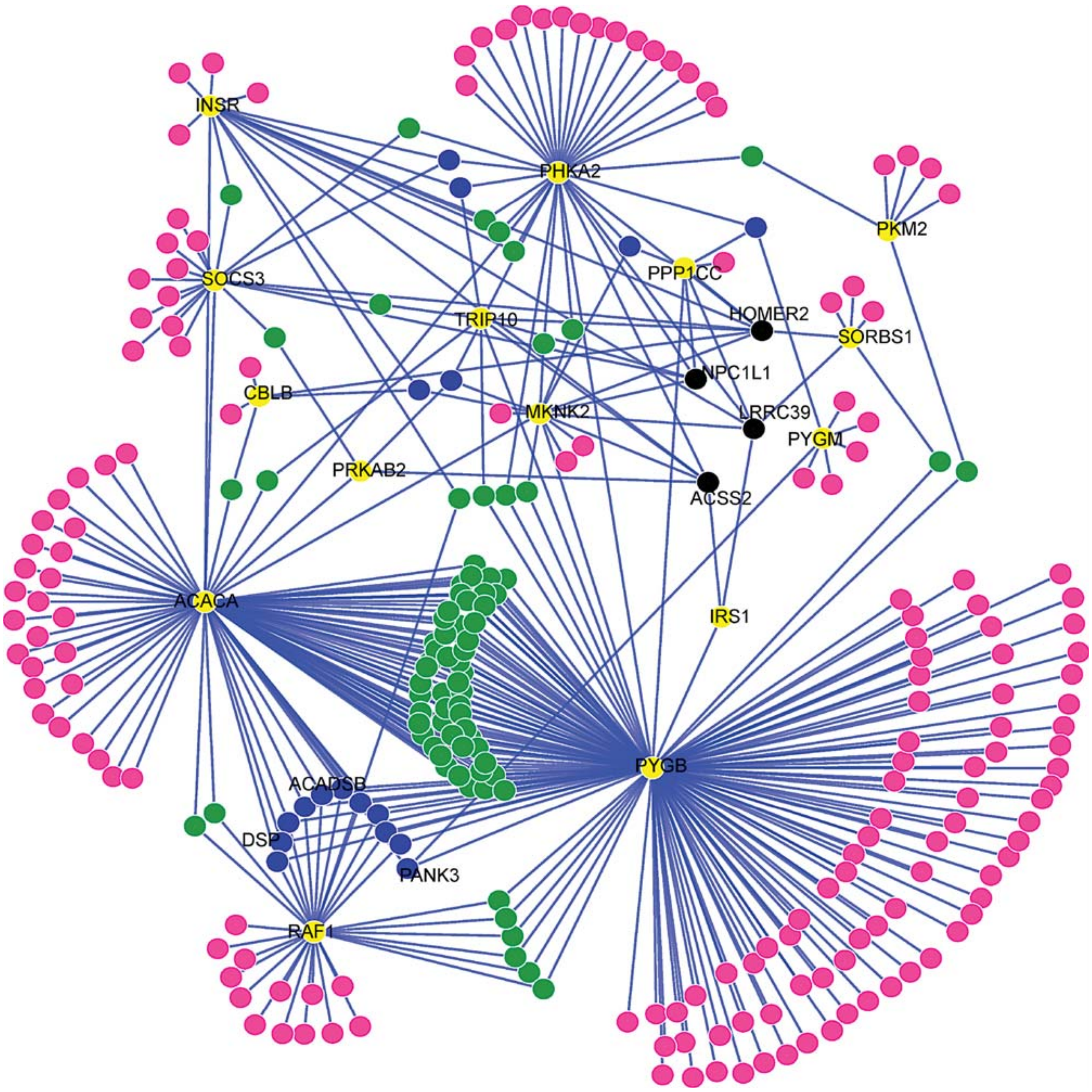
N.D. Leonard; S. Ganesan; S. Calabrese Barton "Rotating ring-disk study of metal-nitrogen-carbon catalyst prepared by high pressure pyrolysis," *ECS Transactions*. 2013;58(1):1681–1689. (2013)

S. Ganesan; N. Leonard; S. Calabrese Barton. "Influence of transition metal on oxygen reduction activity of metal-nitrogen-carbon electrocatalyst," *ECS Transactions*. 2013;58(1):1691–1699. (2013)

# Christina Chan

**Professor** | **krischan@egr.msu.edu** | **517.432.4530** | **428 S. Shaw Lane, Room 1257**




### RESEARCH INTERESTS

Disease mechanisms, system biology, drug delivery, and tissue engineering

### LABS & LOCATION

Cellular & Molecular Laboratory; Integrative Systems and Computational Biology Laboratory, 428 S. Shaw Lane, Room 2125

### GROUP MEMBERS

Aritro Nath, Chun Liu, Ryan Thompson, Daniel Vocelle (co-advised with S. Patrick Walton), Amrita Oak

### WEBSITES

http://www.chems.msu.edu/people/profile/krischan
http://www.egr.msu.edu/changroup/

### PATENTS GRANTED

Sakamoto, J.S.; Tuszynski, M.H.; Gros, T.; Chan, C.; Mehrotra, S. High aspect ratio template and method for producing same for central and peripheral nerve repair. US Patent 8075904, December 13, 2011.

Chan, C. Process for applying a finish to a metal substrate. US Patent 5578347, November 26, 1996.

### CURRENT RESEARCH FOCUS

- ***Network analysis to identify novel targets for cancer.*** The goal is to elucidate the effect of elevated levels of free fatty acids (FFAs), specifically palmitate, on cellular function, given its association with a number of diseases, such as steatosis, obesity, cancer, and Alzheimer's disease. This project addresses the development of a modeling framework that integrates both top-down and bottom-up approaches to generate a phenotype-specific network for cell signaling to help better elucidate how the targets interact to induce a disease phenotype.

- ***Biophysical mechanisms of palmitate-induced signaling and cytotoxicity.*** This project integrates molecular biology, biophysics, and cellular studies with molecular modeling to enhance our understanding of complex biological systems comprising of multiple interacting processes. Specifically, we are studying the endoplasmic reticulum transmembrane protein kinase/endoribonuclease (IRE1), which is activated in response to the Unfolded Protein Response (UPR). This has broad implications on a number of diseases, since UPR is known to be activated in cancers, viral infection, 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.

- ***Role of alignment on axonal growth and myelination.*** Mechanical cues in the cellular environment play important roles in guiding various cell behaviors, such as cell alignment, migration, and differentiation. We hypothesized that the cell senses the physical environment through a more active mechanism, namely, even without external forces the cell can actively apply traction and sense an increased stiffness in the stretched direction and align in that direction.

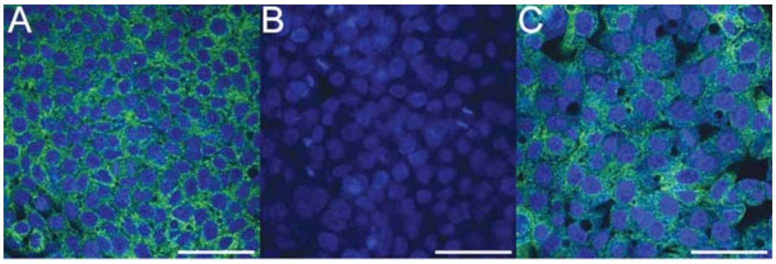



**FIGURE 1.** (*Left*) Sub-network for insulin signaling genes and their neighbor genes in the synergy network. (*Right*) DSP levels. Immuno-fluorescence images of HepG2 cells stained for DSP (green) and cell nuclei (blue) obtained using confocal microscopy [20]. Scale bars represent 50 um. (A) Untreated, control cells grown in regular growth media. (B) Cells treated with PA for 48 hours show decreased DSP levels. (C) Cells treated with PA for 48 hours and recovered in normal growth media for 72 hours show partial recovery of DSP expression.

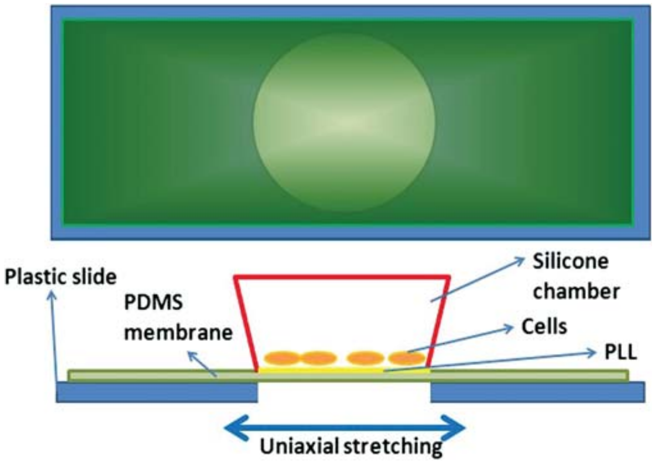



**FIGURE 2.** Design of static pre-stretching device .

## RECENT PUBLICATIONS


Linxia Zhang; Li Liu; Ryan Thompson; Christina Chan. "CREB modulates calcium signaling in cAMP-induced bone marrow stromal cells (BMSCs)," *Cell Calcium*. 2014;56(4):257–268. (2014)

Daniel A. Lynam; Dena Shahriari; Kayla J. Wolf; Phillip A. Angart; Jacob Koffler; Mark H. Tuszynski; Christina Chan; Patrick Walton; Jeffrey Sakamoto. "Brain derived neurotrophic factor release from layer-by-layer coated agarose nerve guidance scaffolds," *Acta Biomaterialia*. 2014. (2014)

Can Huang; Ming Wu; Jun Du; Di Liu; Christina Chan. "Systematic modeling for the insulin signaling network mediated by IRS1 and IRS2," *Journal of Theoretical Biology*. 2014;355:40-52. (2014)

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C. Liu; S. Baek; J. Kim; E. Vasko; R. Pyne; C. Chan. "Effect of static pre-stretch induced surface anisotropy on orientation of mesenchymal stem cells," *Cellular and Molecular Bioengineering*. 2014;7(1):106–121. (2014)

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James C. Costello; . . . NCI DREAM Community, et al., "A community effort to assess and improve drug sensitivity prediction algorithms," *Nature Biotechnology*. 2014;32:1202–12. (2014).

Bansal, M; . . . NCI DREAM Community, et al., "A community computational challenge to predict the activity of pairs of compounds," *Nature Biotechnology*. 2014;32:1213–1222. (2014).

Li Liu; Christina Chan. "The role of inflammasome in Alzheimer's disease." *Ageing Research Reviews*. 2014;15(1):6–15. (2014)

# Martin Crimp

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### RESEARCH INTERESTS

Deformation and fracture of structural materials, diffraction-based electron microscopy of crystalline materials, development of advanced electron microscopy techniques

### LAB & LOCATION

Electron Microscopy, 428 S. Shaw Lane, Rooms 3507 & 3510

### WEBSITE

http://www.chems.msu.edu/people/profile/crimp

### SPECIAL EQUIPMENT AVAILABLE

Scanning electron microscope equipped with *in situ* mechanical test combined with electron backscattered diffraction (EBSD) and high resolution selected area electron channeling pattern (HR-SACP) capabilities for crystallographic analysis

### GROUP MEMBERS

Yang Su, Bret Dunlap

### PATENTS GRANTED

Crimp, M.J.; Wilson, B.A.; Suydam, C.J.; Crimp, M.A. Method of preparing a suspension of particles and related methods. US Patent 5545428, August 13, 1996.

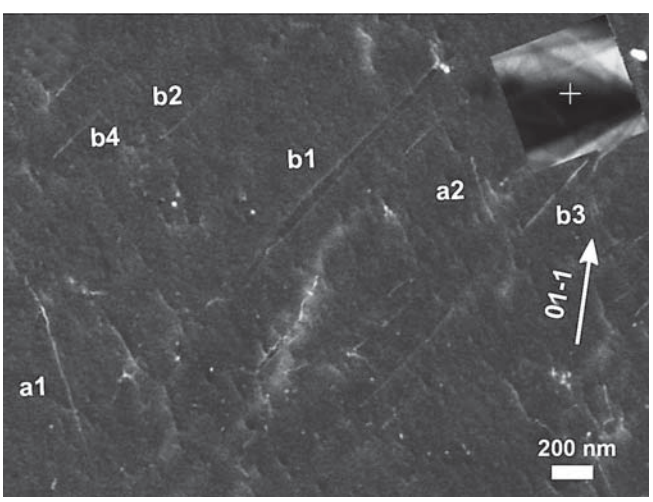



**FIGURE 1.** Deformation structure in interstitial steel showing screw dislocations following 2% plastic strain.

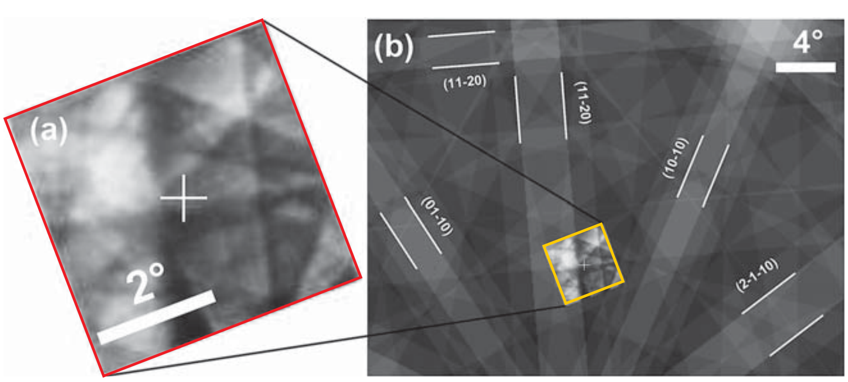



**FIGURE 2.** (A) HR-SACP collected from a sub-micron region of an IF steel, allowing highly accurate imaging of crystal defects. (B) HR-SACP super-imposed on a simulated pattern show imaging conditions in relation to other channeling bands.

### CURRENT RESEARCH FOCUS

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. Ongoing projects include:

- ***Characterization of deformation structures using scanning electron microscopy***, with H. Mansour, J. Guyon, N. Gey, and N. Maloufi.

  Enhancing the performance of metals and alloys used in structural materials 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 of developing SEM approaches to allow the direct imaging and crystallographic characterization of deformation structures in the near surface regions of bulk sample using electron channeling contrast imaging (ECCI) (see Figure 1).

  A key to carrying out these studies is the ability to determine crystal orientation with high accuracy (with 0.1°). While many crystallographic studies in SEM are carried out using EBSD (and we do use this approach extensively in our studies), this approach does not meet the stringent requirements for imaging deformation structures. Rather, selected area channeling patterns (SACPs), historically with spatial resolutions in the range of 10–20 μm, are required for setting up imaging conditions.

  Recently, we have developed a new approach for collecting high resolution selected area channeling patters (HR-SACPs) that spatial resolutions better than 0.5 μm (see Figure 2). In addition to facilitating characterization of deformation structures in fine grain materials, this approach also allows highly accurate misorientation measurements across grain boundaries and dislocation cell walls. Combined with analysis of ECCI image characteristics, this high-accuracy technique allows determination of both geometrically necessary and statistically stored dislocations in deformed structures.

- ***Characterization and modeling of anisotropic deformation in polycrystals***, with T. Bieler, C. Boehlert, P. Eisenlohr, and C. Zambaldi.

  While the mechanisms associated with plastic deformation of single crystals are very well established, the manner in which these mechanisms interact to facilitate the shape changes needed to simultaneously deform the various grains in a polycrystal are not well understood. Critically, if the different grains cannot mutually accommodate imposed strain, performance limiting nucleation of void/cracks may develop. The objective of this research program is to use a combination of advanced characterization techniques in combination with plastic deformation simulations to advance the understanding of polycrystalline deformation and the ability to accurately predict damage nucleation. A critical aspect of polycrystalline deformation is the role that grain boundaries play in limiting the strain transfer from one grain to another.

To study this process in detail, we are currently carrying out nanoindentation experiments and complementary simulations in order to (1) determine the critical parameters for simulating plastic deformation in single crystals and (2) quantify how grain boundaries limit the strain transfer from one grain to the next.

Figure 3 shows an EBSD orientation map with a series of nanoindentations, along with, along with atomic force microscopy (AFM) topography maps of nanoindentation taken close to and far from a grain boundary. It is clear that the topography of the indentations is truncated by the boundary, indicating the boundary resists the transfer of strain from one grain to the other.

Figure 4 shows a series of simulated nanoindentation topographies in comparison with the experimentally measured topography. As the resistance to slip of the grain boundary increased from a from single crystal slip resistance of $\sigma_o = 1.0$ to $\sigma_o = 2.0$, is seen that the amount of topography in the receiving grain decreases and more accurately reflects the experimentally measured topography. The grain boundary slip parameters are found to change for different classes of grain boundaries. These results are being incorporated in to plasticity simulations of polycrystalline arrays to evaluate if the experimentally measured strains can be accurately matched.

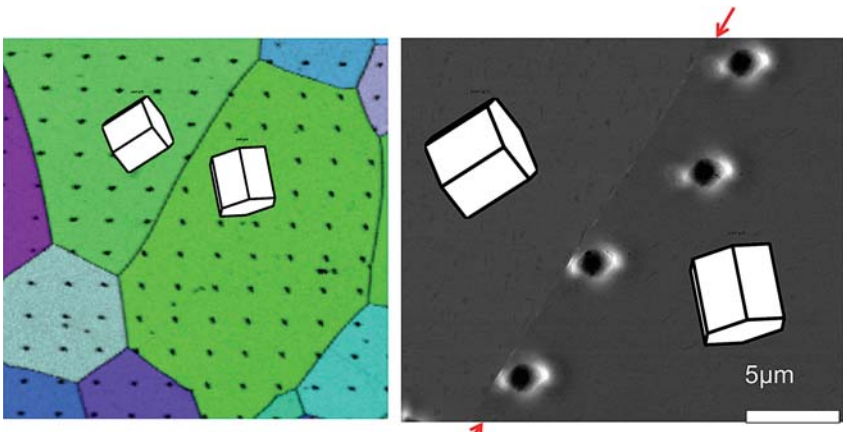
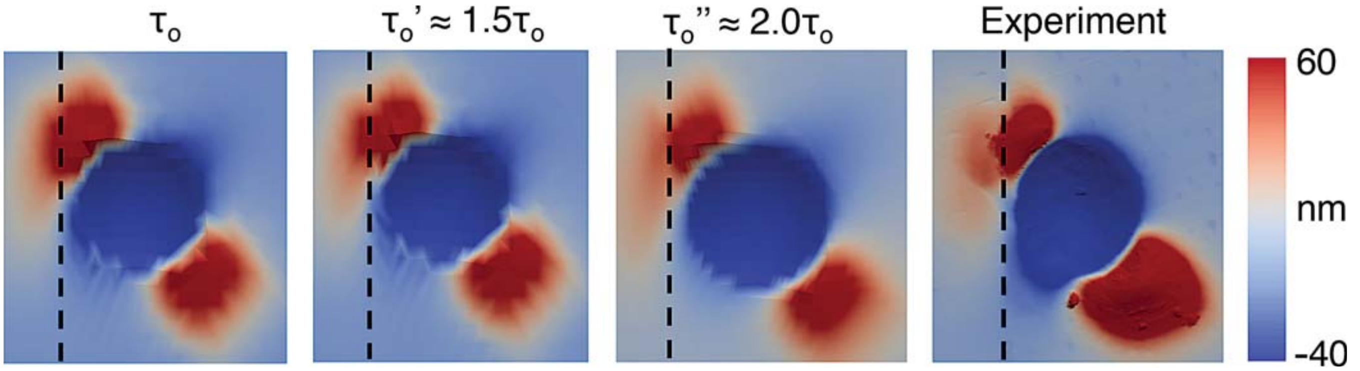



**FIGURE 3.** (*left*) EBSD map of crystal orientations showing nanoindentations. (*right*) High magnification AFM image showing topography changes as the indentations move close to a grain boundary.

**FIGURE 4.** Plastic deformation simulations of nanoindentation topography with varying slip resistance at the grain boundary compared with the experimentally measured topography development.




## RECENT PUBLICATIONS


Yucheng Lan; Feng Lin; Yang Li; Yasmin Dias; Hui Wang; Yuan Liu; Zhen Yang; Haiqing Zhou; Yalin Lu; Jiming Bao; et al. "Gallium nitride porous microtubules self-assembled from wurtzite nanorods," *Journal of Crystal Growth*. 2015;415:139–145. (2015)

H. Li; C.J. Boehlert; T.R. Bieler; M.A. Crimp. "Examination of the distribution of the tensile deformation systems in tension and tension-creep of Ti-6Al-4V (wt.%) at 296 K and 728 K," *Philosophical Magazine*. 2015. (2015)

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T.R. Bieler; P. Eisenlohr; C. Zhang; H.J. Phukan; M.A. Crimp. "Grain boundaries and interfaces in slip transfer," *Current Opinion in Solid State and Materials Science*. 2014;18(4):212–226. (2014)

# Bruce Dale

**University Distinguished Professor | bdale@egr.msu.edu | 517.353.6777 | 3815 Technology Blvd., Suite 115, Lansing, MI**

## RESEARCH INTERESTS

Biofuels, energy and society, sustainability, life cycle assessment

## LAB

Biomass Conversion Research Laboratory

## WEBSITE

http://www.everythingbiomass.org

## SPECIAL EQUIPMENT AVAILABLE

Lab- and pilot-scale equipment for: ammonia fiber expansion (AFEX™) pretreatment of cellulosic biomass, enzymatic hydrolysis and fermentation of cellulose and hemicellulose in pretreated biomass, lignin extraction and purification from biomass

## GROUP MEMBERS

FIXED TERM FACULTY: Professor Venkatesh Balan and Professor Seungdo Kim. POST DOCS: Dr. Leo Sousa. DOCTORAL STUDENTS: Cory Sarks, Saisi Xue, Andrea Orjuela.

## RECENT PATENTS GRANTED (42 TOTAL)

Dale, B.E. et al. Methods for pretreating biomass. US Patent 8968515, March 3, 2015.

Dale, B.E. et al. Methods of hydrolyzing pretreated densified biomass particulates and systems related thereto. US Patent 8945245, February 3, 2015.

Dale, B.E. et al. Process for the treatment of lignocellulosic biomass. US Patent 8771425, July 8, 2014; European Patent 2013368, 2014.

Dale, B.E. et al. Methods for Pretreating Biomass. Mexico Patent 320549, 2014.

Dale, B.E. et al. Pretreated densified biomass products. US Patent 8673031, March 18, 2014.

Dale, B.E. et al. Pretreated densified biomass products and methods of making and using same. Australia Patent 2010289797, 2014.

Dale, B.E. et al. Extraction of solubles from plant biomass for use as a microbial growth stimulant and methods and systems related thereto. Australia Patent 2011201768, 2014.

Dale, B.E. et al. Methods for producing and using densified biomass products containing pretreated biomass fibers. Australia Patent 201320568, 2014.

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Dale, B.E. et al. Pretreated densified biomass products and methods of making and using same. Canada Patent 2760840, 2014; European Patent 2411492, 2014.

## CURRENT RESEARCH FOCUS

Cost-effective conversion of cellulose and hemicellulose in plant biomass to reactive sugars for production of biofuels and bioproducts. Separation and upgrading of lignin streams in plant biomass to fuels and chemicals. Life cycle assessment (LCA) of integrated bioenergy systems to enable sustainable landscape design and sustainable biorefinery processing of biomass.

***Context.*** The U.S. Congress passed the Renewable Fuels Standard (RFS) seven years ago. Since then, biofuels have gone from darling to scapegoat for many environmentalists, policy makers, and the general public. The reasons for this shift are complex and include concerns about environmental degradation, uncertainties about impact on food security, new access to fossil fuels, and overly optimistic timetables. As a result, many people have written off biofuels. However, numerous studies indicate that biofuels, if managed sustainably, can help solve pressing environmental, social and economic problems. In contrast, liquid fuels based on fossil raw materials are likely to come at increasing environmental, social and economic cost.

***Why We Need Biofuels.*** Access to high-quality energy sources is strongly linked to prosperity and human well-being. Economies benefit when they produce biofuels, a dynamic observed in both developed and developing nations. Indigenous biofuel production increases energy security. Producing perennial biofuel feedstocks can improve water and soil quality, biodiversity, and wildlife habitat compared to landscapes dominated by annual crops. Biofuels can also enhance rural employment and food security.

Because photosynthesis consumes $CO_2$ and because some cropping systems can accumulate soil carbon, biofuel production and utilization can be carbon neutral and even reduce net atmospheric $CO_2$. Thus low-carbon energy scenarios developed by diverse organizations foresee wide spread use of biomass for energy. Biomass provides an average of 138 exajoules of primary energy in these scenarios, or about one quarter of total global primary energy. These scenarios use biomass primarily to satisfy energy needs that likely cannot be met by other renewables. For example, aviation and ocean shipping require liquid fuels and liquid fuels are strongly preferred for long-haul trucking. Biofuels are only one part of a sustainable energy portfolio, but it is highly unlikely that we can achieve a sustainable transportation sector without biofuels.

Many materials used by society can be recycled, but fossil fuels cannot. Economic activities based on massive fossil fuel consumption are therefore inherently unsustainable. Extracting and using oil, natural gas, and coal exposes humankind to air and water pollution and to escalating climate challenges. Thus both economic self-interest and ethical considerations require that we develop sustainable alternatives to fossil fuels, including biofuels.

Thus the Biomass Conversion Research Laboratory (BCRL) at MSU is focused on the cost-effective and environmentally-sustainable conversion of plant biomass into fuels and chemicals. We also try to inform policy makers and the general public about the central role of large scale energy use in providing prosperity, and hence the critical need to develop renewable energy systems, including biofuels, to provide long term prosperity. Our work is focused in three primary areas: (1) carbohydrate conversion, (2) lignin conversion and (3) life cycle assessment to assist sustainable biofuel system design and support policy formation.

- ***Carbohydrate utilization.*** We pretreat cellulosic biomass with concentrated ammonia to open up the structure of the plant material and thereby provide easier access of hydrolytic enzymes to produce clean sugar streams for fermentation to fuels and chemicals. Pretreated biomass is valuable both as a biofuel feedstock and an enhanced animal feed, thereby minimizing perceived “food vs. fuel” conflicts.

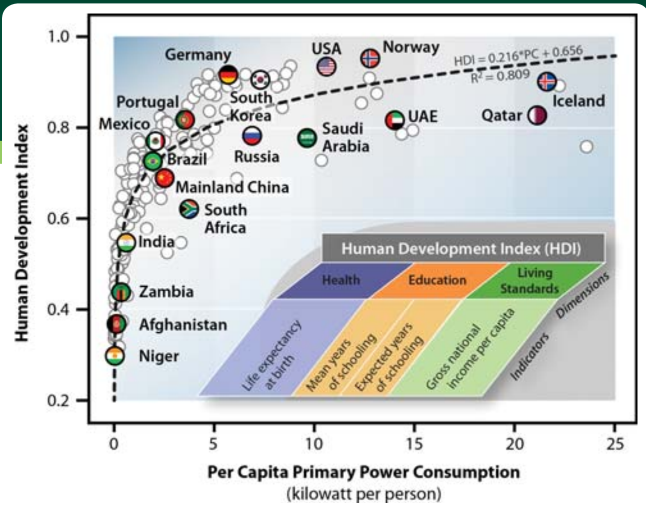


**FIGURE 1.** Human well-being depends strongly on the rate of energy consumption.

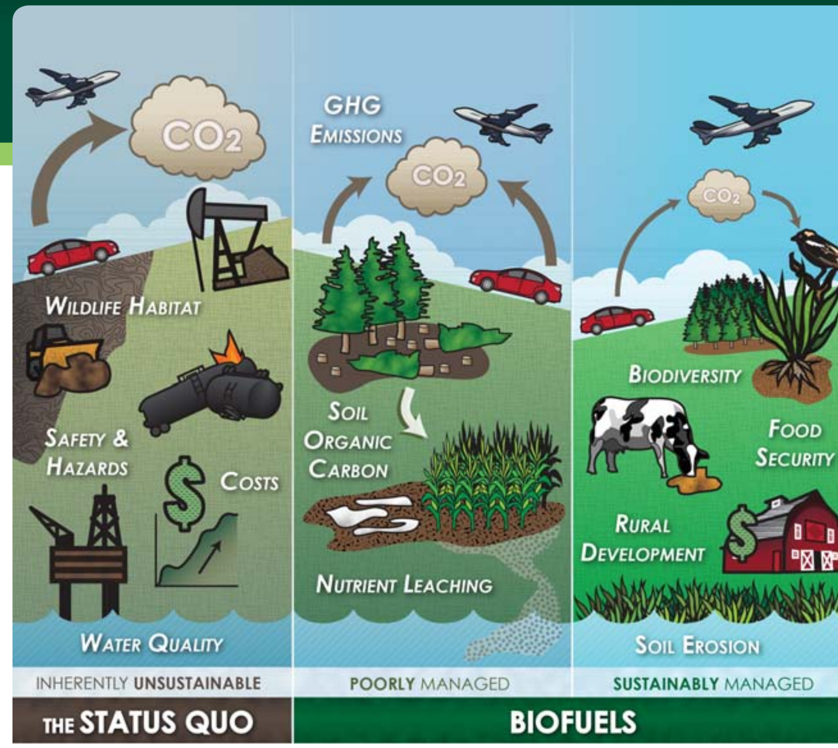


**FIGURE 2.** We can do biofuels well or poorly but the status quo is unsustainable.

- ***Lignin conversion.*** Approximately 20–25% of plant biomass is lignin, a high molecular weight aromatic polymer. It is important to convert lignin into value added products, especially in the current situation where aromatic feedstocks are in short supply. We extract lignin from biomass with liquid ammonia and then fractionate it into various streams depending on differential solubility in ethanol and water. We are exploring various options to add value to these fractionated streams.
- ***Life Cycle Assessment (LCA).*** LCA is the "gold standard" for evaluating the sustainability of products and processes. We use LCA to evaluate integrated biofuel systems (including agricultural biomass production and the "biorefinery" processing operations) and thereby understand how their environmental performance can be improved. Our LCA studies are also the basis by which we attempt to inform policy makers and the public about biofuels.

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Xiadi Gao; Rajeev Kumar; Seema Singh; Blake A. Simmons; Venkatesh Balan; Bruce E. Dale; Charles E. Wyman. "Comparison of enzymatic reactivity of corn stover solids prepared by dilute acid, AFEX™, and ionic liquid pretreatments," *Biotechnology for Biofuels*. 2014;7(1). (2014)

Nirmal Uppugundla; Leonardo Da Costa Sousa; Shishir P.S. Chundawat; Xiurong Yu; Blake Simmons; Seema Singh; Xiadi Gao; Rajeev Kumar; Charles E. Wyman; Bruce E Dale; et al. "A comparative study of ethanol production using dilute acid, ionic liquid and AFEX™ pretreated corn stover," *Biotechnology for Biofuels*. 2014;7(1). (2014)

Bryan D. Bals; Christa Gunawan; Janette Moore; Farzaneh Teymouri; Bruce E. Dale. "Enzymatic hydrolysis of pelletized AFEX™-treated corn stover at high solid loadings," *Biotechnology and Bioengineering*. 2014;111(2):264–271. (2014)

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Bruce E. Dale; Rebecca G. Ong. "Design, implementation, and evaluation of sustainable bioenergy production systems," *Biofuels, Bioproducts and Biorefining*. 2014;8(4):487–503. (2014)

# 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

## WEBSITE

http://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: Zeiss Environmental Scanning Electron Microscope (ESEM) integrated with a Dual-Beam Focused Ion Beam (FIB), X-ray Photoelectron Spectroscopy PerkinElmer 5400, Contact Angle Krusse Dynamic measurement System, Contact Angle Cahn Microbalance , Thermal Analysis TA 2900Instruments (DSC, TGA, TMA, DTA), Rheological Analysis TA Instruments AR2000X Rheometer, AFM-Scanning Probe Microscopy (Nano Scope IV), Nano-Indentation- MTS, Permeability Mocon permeability System (water, $CO_2$, $O_2$), Thermal Conductivity System Anter Unitherm 2022, Ultramictrotomy RMC-MT7, Ultrasoncinator Heilsher 1000W pulsed system, Potentiostat/Galvanostat Measurement Applied Research VMC-2 Versastat System), Inert fabrication Glovebox MBRAUN Unilab 2000/780 Argon Glovebox, Plasma Surface Modification Plasma Sciences 500 Surface Treatment plasma reactor, UV Light Source: Xenon RC 747 HVPS system, Rheometer, TA Instruments AR2000ex, ARES, Viscometer-Brookfield, Netzsch Xenon Flash Thermal conductivity units.

COMPOSITE MATERIALS FABRICATION: Cryo-Mill Mikro-Bantam Model CF, C.W. Brabender 85cc Banbury Mixer, Labram Vacuum Mixing Sys, Sweco Vibro-Energy Grinding Mill, Exact Three Roll Mill, Microwave Synthesis Milestone ETHOS EZ Microwave Labstation, Tetrahedron Programmable Smart Press, 40 ton, Double Daylight, Temp 1000°F, Programmable Temp and Pressure, Leistritz Micro-27 Twin Screw Extruder System And Related Auxiliary Equipment, DSM Research 15 cc Micro-extruder (two units), Killion.75 in Single Screw Extruder, Cincinnati Milacron Sentry 85 Injection Molder, United McGill Autoclave, Research Tool Hot-Melt Prepregger (two units), Research System Resin Transfer Molding

## GROUP MEMBERS

PHD STUDENTS: Yan Li, Deandrea Rollins,Markus Downey, Keith Honaker-Schroeder, Nicholas Kamar, Mariana Batista, Zeyang Yu

## RECENT PATENTS GRANTED (35 TOTAL)

Drzal, L.T.; Do, I.; Monga, A. Method for the preparation of doped single graphene sheets. US Patent 8834959, September 16, 2014.

Drzal, L.T.; Fukushima, H. Expanded graphite and products produced therefrom. US Patent 8501858, August 6, 2013.

Drzal, L.T.; Do, I. Method for preparing metal nanoparticles. WO/2013/049433 PCT/US2012/057694.

## CURRENT RESEARCH FOCUS

***Nanostructuring of multifunctional graphene nano-platelet 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 super-capcitors.*** 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 nanostructuring of graphene nanoplatelets in the anode to improve capacity, re-charging rate, and durability.

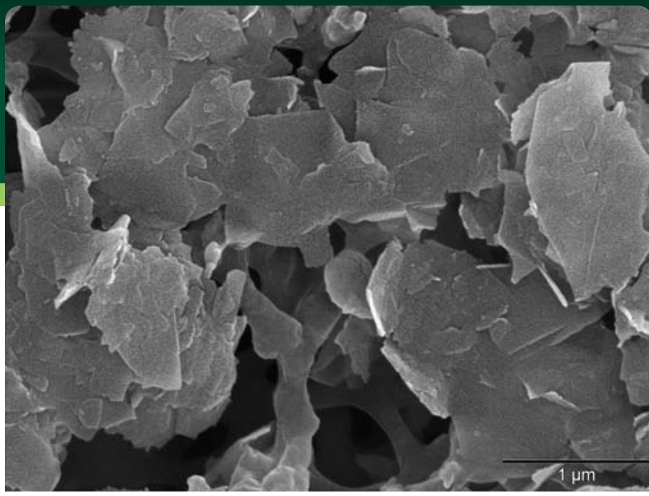


**FIGURE 1.** Graphene nanoplatelets.

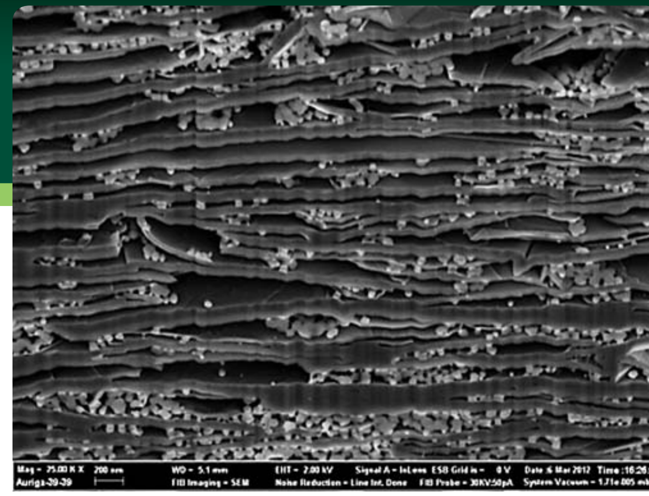

**FIGURE 2.** Composite impact resistance enhancement with selective placement of nanoparticles.

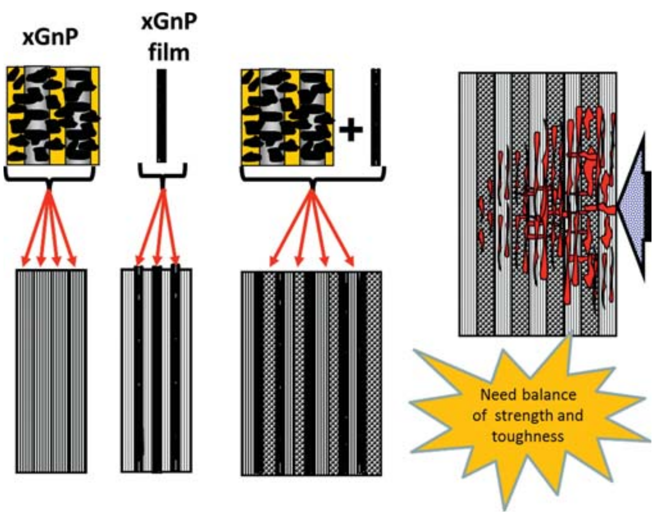


**FIGURE 3.** Nanostructured Li-ion battery anode.

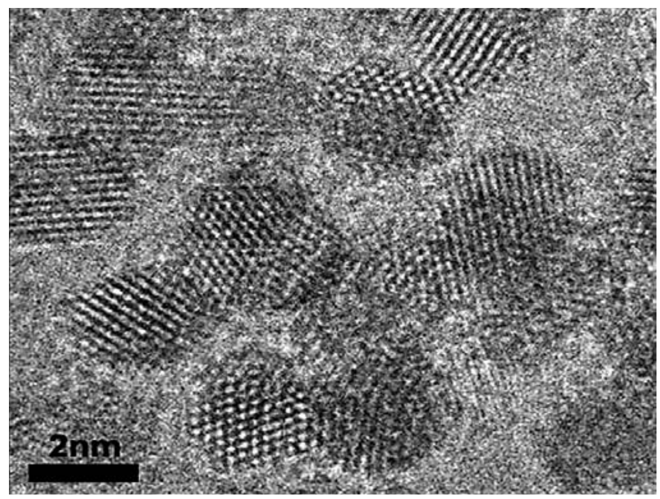


**FIGURE 4.** 2nm Platinum nanoparticles synthesized on the basal plane of graphene nanoplatelets.

- ***Multifunctional materials for blast and impact resistance.*** 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.

  SPONSOR: U.S. Army, TARDEC.

## RECENT PUBLICATIONS

Wenzhen Qin; Frederic Vautard; Lawrence T. Drzal; Junrong Yu. “Mechanical and electrical properties of carbon fiber composites with incorporation of graphene nanoplatelets at the fiber-matrix interphase,” *Composites Part B: Engineering*. 2015;69:335–341. (2015)

Wenzhen Qin; Frederic Vautard; Per Askeland; Junrong Yu; Lawrence Drzal. “Modifying the carbon fiber-epoxy matrix interphase with silicon dioxide nanoparticles,” *RSC Advances*. 2015;5(4):2457–2465. (2015)

Nicholas T. Kamar; Mohammad Mynul Hossain; Anton Khomenko; Mahmood Haq; Lawrence T. Drzal; Alfred Loos. “Interlaminar reinforcement of glass fiber/epoxy composites with graphene nanoplatelets,” *Composites Part A: Applied Science and Manufacturing*. 2015;70:82–92. (2015)

Markus A. Downey; Lawrence T. Drzal. “Toughening of aromatic epoxy via aliphatic epoxy copolymers,” *Polymer* (United Kingdom). 2014;55(26):6658–6663. (2014)

Fuzhong Wang; Lawrence T. Drzal; Yan Qin; Zhixiong Huang. “Mechanical properties and thermal conductivity of graphene nanoplatelet/epoxy composites,” *Journal of Materials Science*. 2014. (2014)

Inhwan Do; Lawrence T. Drzal. “Ionic liquid-assisted synthesis of pt nanoparticles onto exfoliated graphite nanoplatelets for fuel cells,” *ACS Applied Materials and Interfaces*. 2014;6(15):12126–12136. (2014)

Huang Wu; Lawrence T. Drzal. “Effect of graphene nanoplatelets on coefficient of thermal expansion of polyetherimide composite,” *Materials Chemistry and Physics*. 2014;146(1–2):26–36. (2014)

V. Cech; A. Knob; H.-A. Hosein; A. Babik; P. Lepcio; F. Ondreas; L.T. Drza. “Enhanced interfacial adhesion of glass fibers by tetravinylsilane plasma modification,” *Composites Part A: Applied Science and Manufacturing*. 2014;58:84–89. (2014)

Saswata Bose; Lawrence T. Drzal. “Role of thickness and intercalated water in the facile reduction of graphene oxide employing camera flash,” *Nanotechnology*. 2014;25(7). (2014)

Jinglei Xiang; Lawrence T. Drzal. “Improving thermoelectric properties of graphene/polyaniline paper by folding,” *Chemical Physics Letters*. 2014;593:109–114. (2014)

Inhwan Do; Lawrence T. Drzal. “Room temperature ionic liquids for size control of noble metal nanoparticles on carbon supports,” *Carbon*. 2014;75:43–55. (2014)

Gomatheeshwar Pitchiaya; Lawrence Drzal. “ABA and ABC type thermoplastic elastomer toughening of epoxy matrices,” *International SAMPE Technical Conference*. 2014. (2014)

# Philip Eisenlohr

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

## RESEARCH INTERESTS

Computational materials science, mechanics of microstructured materials, crystal plasticity

## LAB & LOCATION

Computational Materials Mechanics, 428 S. Shaw Lane, Room 1260

## WEBSITE

http://researchgroups.msu.edu/cmm

## SPECIAL EQUIPMENT AVAILABLE

Dedicated computer clusters at the MSU High Performance Computing Center

## GROUP MEMBERS

Tias Maiti, Aritra Chakraborty, Zhuowen Zhao, Chen Zhang, David Smiadak, Siddharth Rath

## CURRENT RESEARCH FOCUS

***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 mesoscopic 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.

Examples for ongoing research are:

- ***Virtual deformation lab for materials with complex micro-structures.*** The microstructure of materials has a profound influence on their mechanical properties and performance. For complex microstructures that contain largely different phase constituents, such as advanced steel grades or Ti-alloys, predictions of material behavior based on analytical approaches, which necessarily make simplifying assumptions, tend to have limited reliability. Therefore, the numerical simulation of the intricate interactions occurring within the materials is essential. Our group actively improves the methodologies to accelerate such calculations and develops them into a "virtual deformation

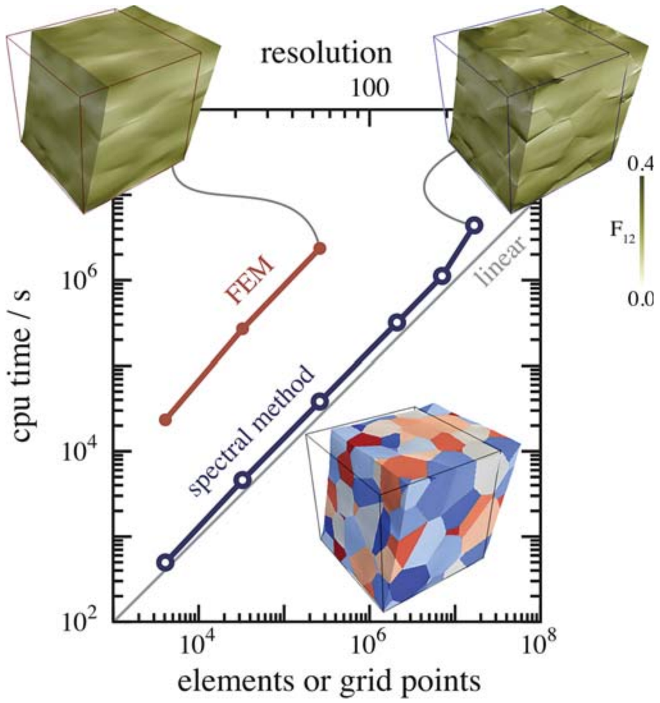


**FIGURE 1.** Speed-up of about 50 to solve shear deformation of a polycrystalline aggregate (*bottom right*) by the spectral method compared to conventional finite element method (FEM). Resulting strain (deformation gradient) field shown in top insets.

laboratory" that allows to test materials in the computer based on knowledge of their microstructure. The method used to solve the boundary value problem in the virtual lab is substantially faster than the typically employed finite element method (FEM). This makes it possible to statistically screen the propensity of microstructures for hot spot formation where performance-limiting damage might nucleate. In addition, the fast property simulation can be used to design optimized materials before even synthesizing them.

- ***Systematic identification of constitutive parameters for crystal plasticity models of non-cubic metal alloys.*** The integration of computational modeling into process development and design continues to accelerate due the potential shortened development times, cost savings, and enhanced reliability. At the fundamental level, the controlling factors in the mechanical behavior of structural metals are the resistance of dislocations to slip, i.e., the critical resolved shear stress for the motion of dislocations, and the concurrent structural evolution (e.g., work hardening). Thus, in order to accurately describe the deformation, possible damage nucleation, and fracture behavior of the polycrystalline arrays that make up structural components, it is necessary to have a sound model with physical deformation processes involved and accurate values for the adjustable parameters that enter such models. Determining these constitutive parameters proved difficult in technologically relevant materials of low crystal symmetry, such as Mg-alloys, Ti-alloys, or lead-free solders based on Sn.

We will try to apply a newly developed approach to determine parameters of the constitutive description in a relatively rapid and cost-effective manner by sphero-conical nano-indentation into a sufficiently large number of different crystal orientations at the surface of polycrystalline samples. Atomic force microscopy is then used to measure the topography around these indents, which is a strong function of the crystal orientation and the specific local activity of different slip systems. Crystal plasticity finite element simulation of the indentation process is then carried out with varying constitutive parameters until an optimal match is achieved between the measured and simulated topographies in several different indents on crystals with different orientations/topographies. This method is effective because the axisymmetric sphero-conical indentation geometry causes many different slip systems to operate at different rates and along different strain paths depending on the material location beneath the indent.

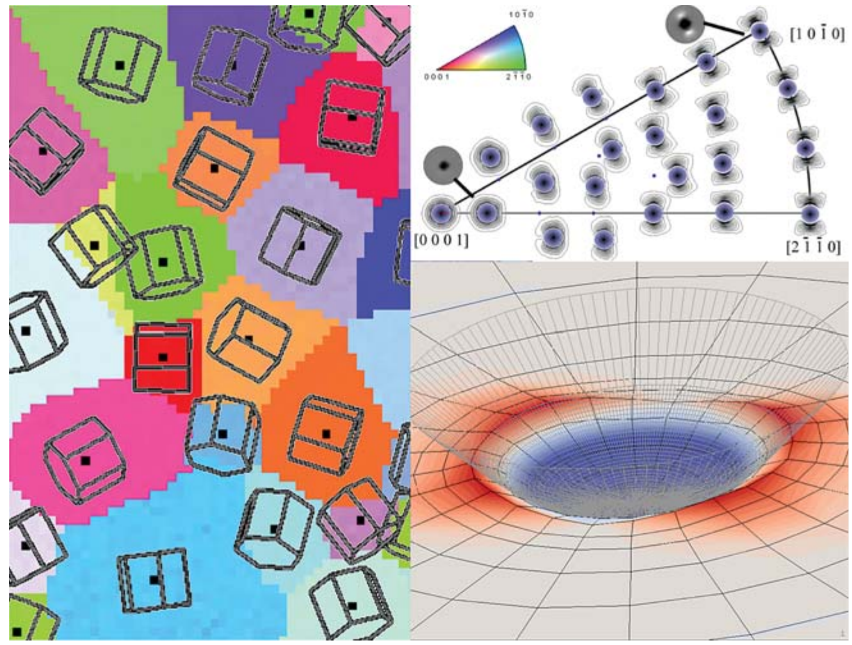


**FIGURE 2.** Grain structure on a polished surface indicated by crystal orientation-dependent color (*left*). Simulated (*bottom right*) surface topography resulting from indenting in differently oriented grains compared to two measured topographies (*top right*).

## RECENT PUBLICATIONS

C. Zhang; H. Li; P. Eisenlohr; W. Liu; C.J. Boehlert; M.A. Crimp; T.R. Bieler. "Effect of realistic 3D microstructure in crystal plasticity finite element analysis of polycrystalline Ti-5Al-2.5Sn," *International Journal of Plasticity*. 2015;69:21–35. (2015)

W. Blum; J. Dvořák; P. Král; P. Eisenlohr; V. Sklenička. "What is "stationary" deformation of pure Cu?" *Journal of Materials Science*. 2014;49(8):2987–2997. (2014)

W. Blum; J. Dvořák; P. Král; P. Eisenlohr; V. Sklenička. "Effect of grain refinement by ECAP on creep of pure Cu," *Materials Science and Engineering A*. 2014;590:423–432. (2014)

Thomas R. Bieler; Scott C. Sutton; Bret E. Dunlap; Zackery A. Keith; Philip Eisenlohr; Martin A. Crimp; Brad L. Boyce. "Grain boundary responses to heterogeneous deformation in tantalum polycrystals," *JOM*. 2014;66(1):121–128. (2014)

C. Reuber; P. Eisenlohr; F. Roters; D. Raabe. "Dislocation density distribution around an indent in single-crystalline nickel: Comparing nonlocal crystal plasticity finite-element predictions with experiments," *Acta Materialia*. 2014;71:333–348. (2014)

Masahiko Demura; Dierk Raabe; Franz Roters; Philip Eisenlohr; Ya Xu; Toshiyuki Hirano; Kyosuke Kishida. "Slip system analysis in the cold rolling of a $Ni_3Al$ single crystal," *Materials Science Forum*. 2014;783–786:1111–1116. (2014)

T.R. Bieler; P. Eisenlohr; C. Zhang; H.J. Phukan; M.A. Crimp. "Grain boundaries and interfaces in slip transfer," *Current Opinion in Solid State and Materials Science*. 2014;18(4):212–226. (2014)

# David Hodge

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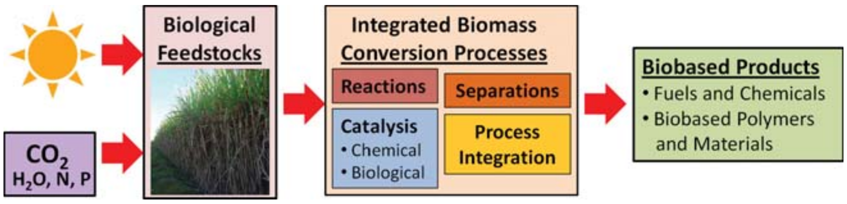


**FIGURE 1.** Scope of the research program in the Hodge laboratory.

### RESEARCH INTERESTS

Bioenergy, biomass conversion, lignin, bio-based products

### LAB LOCATION

28 Trout Building

### WEBSITE

http://www.chems.msu.edu/groups/hodge/

### GROUP MEMBERS

Ryan Stoklosa, Muyang Li, Jacob Crowe, Thanaphong Phongpreecha, Lisaura Maldonado, Dhruv Gambhir

### PATENTS GRANTED

Hodge D.B.; Hegg E.L.; Li Z.; Bhalla A.; Bansal N. Multi-ligand Metal Complexes and Methods of Using Same to Catalytically Pretreat Lignocellulosic Biomass. US Provisional Patent, 2014.

### CURRENT RESEARCH FOCUS

***Conversion of plant-derived biomass to renewable fuels, chemicals, polymers, and materials.***

The long-term sustainability of human civilization will ultimately require non-fossil sources of both energy and carbon as well as the technologies for their effective capture, storage, and conversion. Non-food plant biomass offers an immense reservoir of reduced carbon that can be utilized for renewable fuels, chemicals, polymers, and materials if technological and economic barriers can be overcome. Work in the Hodge Laboratory is focused on overcoming these barriers by addressing fundamental and applied problems associated with the conversion of plant-derived biomass to renewable bioproducts through integrated biochemical and chemical catalytic conversion routes.

- ***Catalytic oxidation of lignin to improve hydrolysis of woody biomass.*** In nature, microbes successfully degrade plant cell walls using a variety of oxidative approaches. These strategies include the release of reactive oxygen species produced by redox-active metals and metalloenzymes. As co-PI on a project funded by the DOE GLBRC since 2010, we are investigating applying abiotic catalytic oxidative treatments that mimic certain features of these successful biological approaches. Ongoing work is focused on understanding the mechanisms by which enzymatic hydrolysis is improved and developing more effective and economic catalytic systems. Select highlights from this work are presented in Figure 2.

- ***Understanding the plant cell wall porosity and polysaccharide accessibility.*** In work funded by NSF CBET beginning 2014 we are investigating the role that the non-covalent forces exerted by plant cell wall polymers within nanoscale cell wall pores have on a number of important phenomena influencing plant cell wall deconstruction and how these properties evolve during pretreatment and hydrolysis that lead to outcomes of improved polysaccharide conversion. Specifically this involves the role of surface properties in influencing: (1) water infiltration into the cell wall and cell wall swelling, (2) cellulolytic enzyme accessibility to binding sites within the cell wall, and (3) enzyme

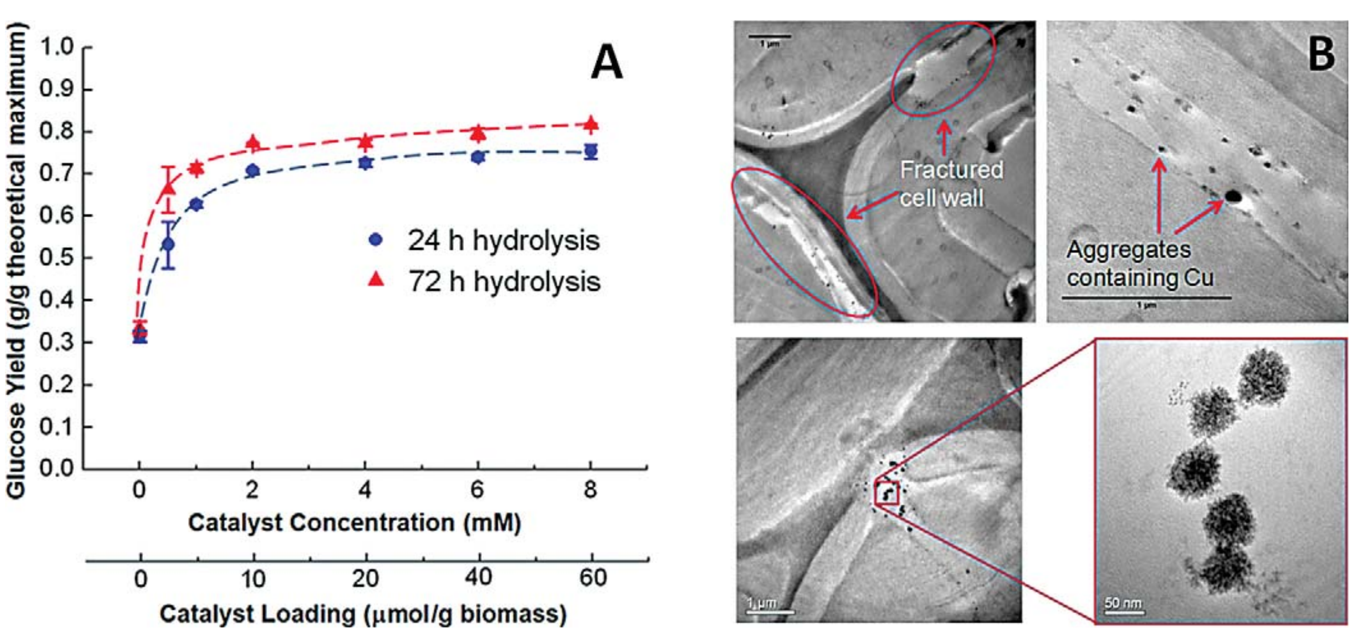


**FIGURE 2.** Demonstration of (A) improved enzymatic hydrolysis yields using catalyzed oxidative delignification and (B) plant cell wall disruption and localization catalyst-containing nanoclusters within the cell wall as validated by EDS.

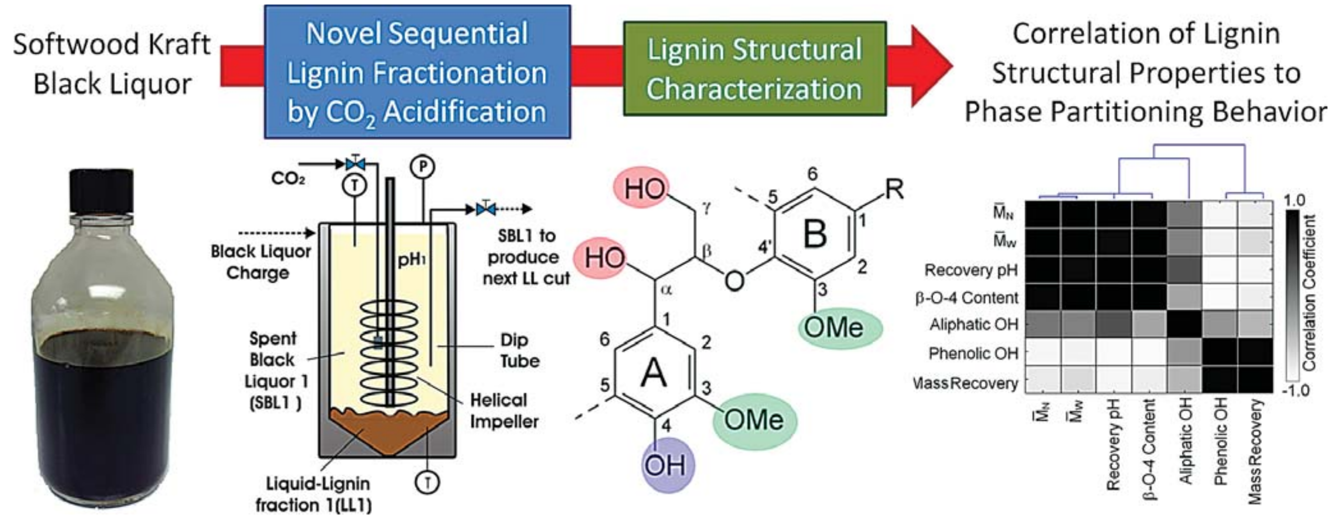


**FIGURE 3.** Solubility-based fractionation of alkali-solubilized lignin. *Green Chem.*, 2013, 15, 2904–2912.

binding to chemically and physically modified surfaces within the cell wall. For this, we propose to investigate a new paradigm for understanding plant cell wall recalcitrance, specifically that the limitations of cell wall porosity and inaccessible surface area to enzymes, can be best investigated in the context of understanding the plant cell wall matrix as a water-swellable hydrogel and understanding the porosity in the context of hydrogel swelling due to the opposing forces of water swelling versus the resistance of the plant cell wall matrix to swelling imparted by lignification.

- ***Relating plant cell wall biopolymer properties to phase partitioning behavior.*** Currently, the North American forest products industry is undergoing a period of decreased profitability and consolidation which presents the opportunity for product diversification through the integration of technologies for biobased fuels and chemicals with existing processes and infrastructure. One research thrust has been targeted at technologies for hemicellulose and lignin extraction, recovery, and catalytic conversion to add value to the forest products industry. This includes research that seeks to understand how the properties of cell wall biopolymers solubilized during alkaline pretreatments or pulping processes impact their processing behavior and how this understanding can be exploited by solubility-based separations processes to extract more value from alkaline pulping or alkaline pretreatment process streams. Highlights from this work include publications on understanding the processing behavior of xylans and lignin during alkaline pretreatments, linking lignin structural properties to its solubility and phase partitioning behavior in a novel pH-based fractionation process involving sequential $CO_2$ acidification and separation (Figure 3), and the novel identification that up to 20% of soluble biopolymers in hardwood Kraft black liquors can be recoverable polysaccharides that can be integrated with a butanol fermentation. Other work is directed at the conversion of lignins derived from biorefinery and forest products industry process streams to phenolic acid and aldehyde monomers that may be used for higher value applications including renewable polymers that displace petroleum-derived polymers.

## RECENT PUBLICATIONS


Felipe Scott; Muyang Li; Daniel L. Williams; Raúl Conejeros; David B. Hodge; Germán Aroca. “Corn stover semi-mechanistic enzymatic hydrolysis model with tight parameter confidence intervals for model-based process design and optimization,” *Bioresource Technology*. 2015;177:255–265. (2015)

Ryan J. Stoklosa; David B. Hodge. “Fractionation and Improved Enzymatic Deconstruction of Hardwoods with Alkaline Delignification,” *Bioenergy Research*. 2015. (2015)

Rasika L. Kudahettige-Nilsson; Jonas Helmerius; Robert T. Nilsson; Magnus Sjöblom; David B. Hodge; Ulrika Rova. “Biobutanol production by Clostridium acetobutylicum using xylose recovered from birch Kraft black liquor,” *Bioresource Technology*. 2015;176:71–79. (2015)

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Tongjun Liu; Daniel L. Williams; Sivakumar Pattathil; Muyang Li; Michael G. Hahn; David B. Hodge. “Coupling alkaline pre-extraction with alkaline-oxidative post-treatment of corn stover to enhance enzymatic hydrolysis and fermentability,” *Biotechnology for Biofuels*. 2014;7(1). (2014)

Daniel L. Williams; David B. Hodge. “Impacts of delignification and hot water pretreatment on the water induced cell wall swelling behavior of grasses and its relation to cellulolytic enzyme hydrolysis and binding,” *Cellulose*. 2014;21(1):221–235. (2014)

Yogender Kumar Gowtham; Kristen P. Miller; David B. Hodge; J. Michael Henson; Sarah W. Harcum. “Novel two-stage fermentation process for bioethanol production using Saccharomyces pastorianus,” *Biotechnology Progress*. 2014;30(2):300–310. (2014)

Trey K. Sato; Tongjun Liu; Lucas S. Parreiras; Daniel L. Williams; Dana J. Wohlbach; Benjamin D. Bice; Irene M. Ong; Rebecca J. Breuer; Li Qin; Donald Busalacchi; et al. “Harnessing genetic diversity in saccharomyces cerevisiae for fermentation of xylose in hydrolysates of alkaline hydrogen peroxide-pretreated biomass,” *Applied and Environmental Microbiology*. 2014;80(2):540–554. (2014)

# Krishnamurthy Jayaraman

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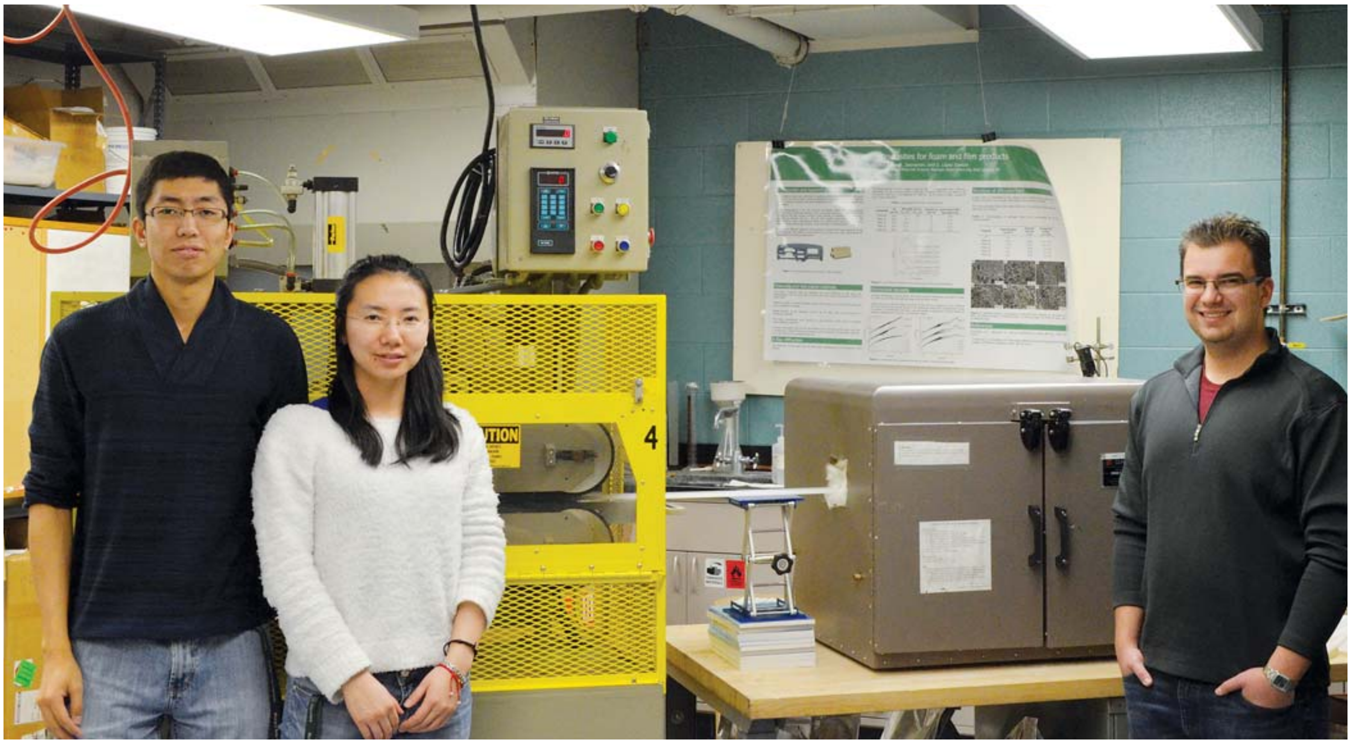

**FIGURE 1.** Drawing apparatus: A belt puller draws the polymer billet from the oven through a converging die.

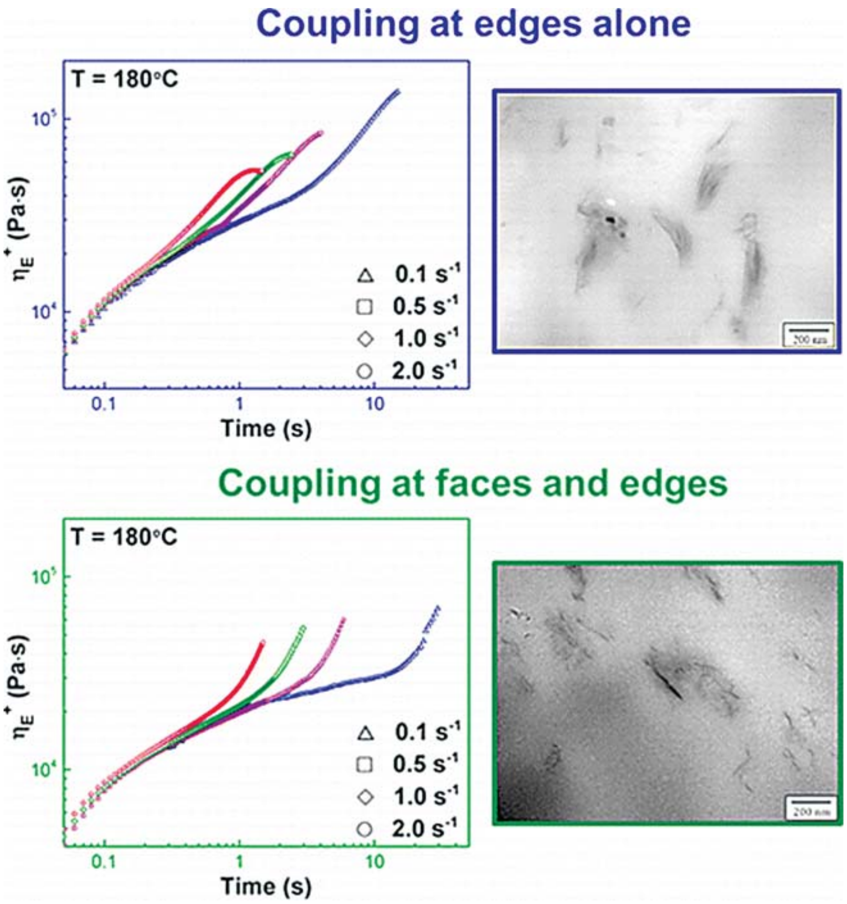


**FIGURE 2.** Reactive coupling at the interface produces finer dispersions and strain hardening in uniaxial extensional flow of polymer-layered silicate nanocomposites—more so with both coupling at faces and edges.

## RESEARCH INTERESTS

Polymer composites processing and rheology. Dr. Jayaraman's research interests and expertise are processing, rheology, and microstructure development in polymer composites, polymer nanocomposites, foams, and porous composites, thermoplastic olefin blends (TPO), elastomers, thermoplastic foams and thermoplastic vulcanizate blends (TPV). This research is aimed at developing processing strategies and chemical treatment methods with coupling agents for rheology modification and microstructure development during melt processing and solid-state processing.

## WEBSITE

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

## GROUP MEMBERS

CURRENT PHD STUDENTS: Weijie Ren, Xinting Lin, Christopher J. Hershey. RECENT PHD GRADUATES: Amit K. Chaudhary (Dow Chemical Co. Midland, MI), Tanmay J. Pathak (A. Schulman Inc., Akron, OH), Rahul H. Rane (Tata Autocomp Systems, Pune, India).

## SPECIAL EQUIPMENT AVAILABLE

TA ARES rheometer with an SER extensional flow fixture for melts, Dynisco capillary rheometer, Polylabs torque rheometer with a Banbury mixer attachment.

## PATENTS

Iyer, S.; Drzal, L.T.; Jayaraman, K. Method for fiber coating with particles. US Patent 5123373, June 23, 1992.

Iyer, S.; Drzal, L.T.; Jayaraman, K. Method coating fibers with particles by fluidization in a gas. US Patent 5102690, April 7, 1992.

Jayaraman, K.; Pathak, T.J.; Chaudhary, A.K. US Patent Application No.12/780,461. Novel Nanocomposites and Nanocomposite Foams and Methods and Products Related to Same. Filed May 14, 2010 and published December 9, 2010. (Pending)

## CURRENT RESEARCH FOCUS

The Polymer Composites Processing and Rheology Research Group at Michigan State University is engaged in the following research projects currently with support and collaboration from ExxonMobil Chemical Co., BASF Battery Materials Division, the Michigan Initiative for Innovation and Entrepreneurship (MIIE), Petoskey Plastics and Eovations LLC.

- Nonlinear rheology of polyamide-based TPVs for extrusion and film blowing
- High-performance additives with nanoparticles for masking film in paint ovens
- Die-drawing of porous polymer composite membranes for battery separators
- Modeling of expanding foam flow due to reaction in heated mold cavities

- ***High-performance additives with nanoparticles for polyolefin films.*** Polymer nanocomposites with layered silicates have two different types of interface sites: edges with hydroxyl groups and gallery faces with oxygen atoms. The polymer-particle interface at either site may be strengthened by silane coupling agents. Effects of reactive coupling by the silane and a long-chain polymeric compatibilizer at different interface sites have been investigated on the morphology and rheology of polypropylene nanocomposites in the melt-compounded state. The resulting state of dispersion and uniaxial extensional viscosity behavior are shown in Figure 2.

  New masterbatch additives have been developed that may be compounded with bulk polyolefins and used in film blowing to produce films with good tensile strength and tear strength while also having much improved barrier to water vapor.

- ***Porous polypropylene composite products.*** High levels of molecular orientation can be produced in semi-crystalline polymers by solid phase processes such as roll-drawing and die-drawing at elevated temperatures below the melting temperature. Die-drawing of particulate-filled polyolefins at elevated temperatures was developed recently to produce expanded and oriented particulate composites that are lighter and stronger after processing. The thickness of the slabstock produced so far by die-drawing has been 2 mm or more for construction materials. The die-drawing process is now being applied to produce much stronger porous sheets or membranes: one application area for such membranes is as separators in batteries.

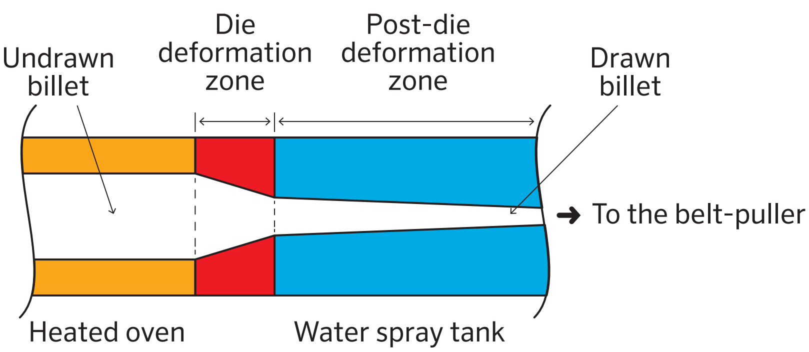


**FIGURE 3.** Die-drawing of extruded billets through a heated die may be used to produce a highly oriented and expanded or stronger and lighter product.

## RECENT PUBLICATIONS


Rahul H. Rane; Krishnamurthy Jayaraman; Kevin L. Nichols; Thomas R. Bieler; Michael H. Mazor. "Evolution of crystalline orientation and texture during solid phase die-drawing of PP-talc composites," *Journal of Polymer Science, Part B: Polymer Physics*. 2014;52(23):1528–1538. (2014)

Carlos A. Diaz; Yining Xia; Maria Rubino; Rafael Auras; Krishnamurthy Jayaraman; Joseph Hotchkiss. "Fluorescent labeling and tracking of nanoclay," *Nanoscale*. 2013;5(1):164–168. (2013)

K. Jayaraman; C.J. Hershey. "Modeling polyurethane foam flow in a mold with constricted vents," Annual Technical Conference–ANTEC, *Conference Proceedings*. 2013;3:1847–1849. (2013)

# Wei Lai

Assistant Professor | laiwei@msu.edu | 517.355.5126 | 428 S. Shaw Lane, Room 3524

## RESEARCH INTERESTS

Advanced materials and electroanalytical methods for energy conversion and storage technologies

## LAB LOCATION

428 S. Shaw Lane, Room 3532

## WEBSITE

http://www.egr.msu.edu/~laiwei

## GROUP MEMBERS

Rengarajan Shanmugam, Matthew Klenk

## CURRENT RESEARCH FOCUS

Research in our lab has 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 and 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. 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. A brief description of ongoing and new research projects in our lab is given below.

- ***Structure and dynamics of Lithium garnet oxides.*** (Figure 1.) Liquid electrolytes in the state-of-the-art Li-ion batteries contain volatile and flammable organic solvents, which has raised safety concerns over the wide adoption of these batteries in large-scale automotive, aeronautic, and stationary applications. Solid electrolytes, i.e., SIC, with high ionic conductivity and good chemical/electrochemical stability could potentially revolutionize the electrode and cell designs and provide superior safety in batteries.

  We are investigating a prototypic series of SIC materials, lithium garnet oxides $Li_{7-x}La_3Zr_{2-x}Ta_xO_{12}$ ($x$ = 0–2). The framework of the materials is composed of $LaO_8$ dodecahedra and TaO6 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. The scientific goal of our research is to understand structure and dynamics of lithium disorder and their effect on lithium ionic conduction. This work is supported by the Division of Materials Research of National Science Foundation.

- "***Bi-functional" electrode materials for Na-ion batteries.*** (Figure 2.) 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 1,000 times more abundant than lithium in earth's crust and sea, and sodium resources are considered practically unlimited. We are studying a class of SMIEC materials, $Na_{2x}(Ni_xTi_{1-x})O_2$, as electrodes for Na-ion batteries. The structure consists of a layered framework of $NiO_6$ and $TiO_6$ octahedra and Na guests in two different cages, i.e., edge and face-shared $NaO_6$ prisms. Since their compositions include both the high redox-potential transition metal element Ni, and the low redox-potential transition metal element Ti, they can be utilized as either a cathode or an anode, i.e., "bi-functional." We have demonstrated the "bi-functionality" of these materials and are currently investigating the relationship between their structures and electrochemical properties.

- ***Chemical bonding, structure and dynamics of thermoelectric materials.*** (Figure 3.) Currently around two-thirds of energy produced in U.S. is rejected mainly in the form of waste heat. Such unused heat can be recovered by thermoelectric processes that directly convert thermal energy directly into electricity.

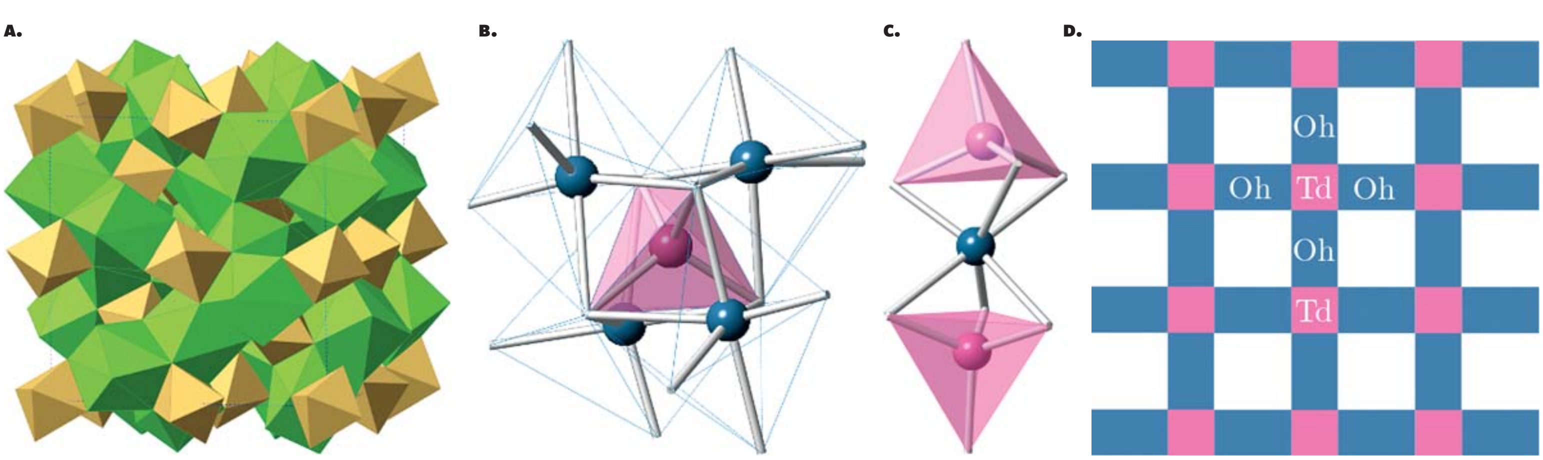


**FIGURE 1.** (A) La-Ta-O framework, (B) Td-Li, (C) Oh-Li, (D) 2D schematic.

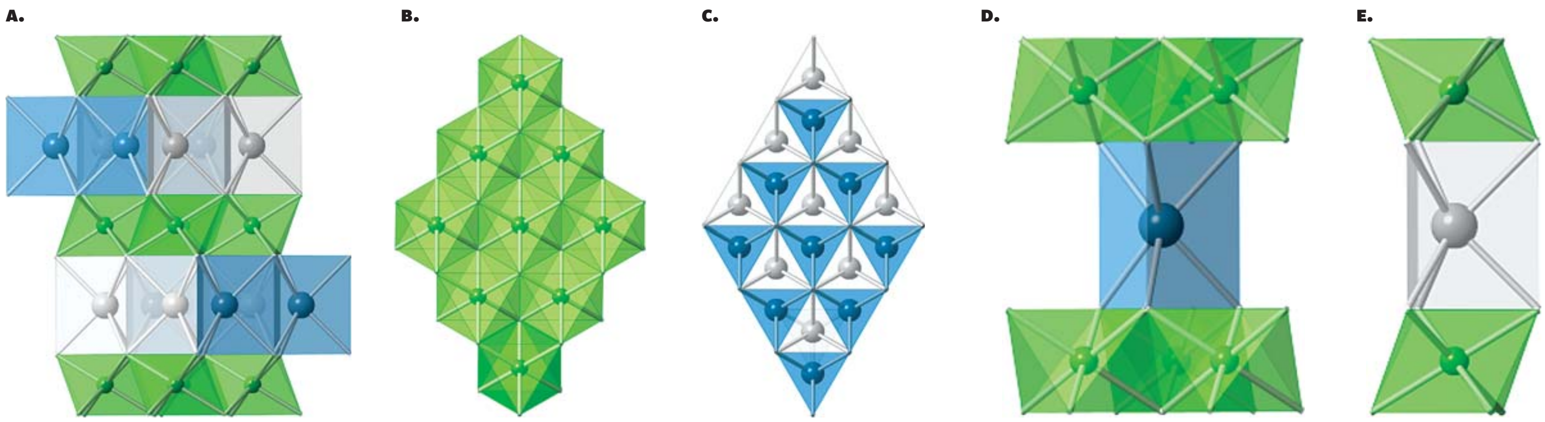


**FIGURE 2.** (A) $Na_{2x}(Ni_xTi_{1-x})O_2$, (B) $[(Ni^{2+}, Ti^{4+})O_2]$, (C) $Na^e$ and $Na^+$ guests, (D) framework-guest interaction: edge, (E) framework-guest interaction: face.

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 $Cu_{12}Sb_4S_{13}$ containing earth-abundant and environmentally friendly elements. The structure consists of a 3D framework of $CuS_4$ tetrahedra and $SbS_3$ polyhedra. Another type of Cu atoms ($Cu^{12e}$) behave as rattling guests inside a cage formed by three S and two Sb atoms. The interaction between $Cu^{12e}$ 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 $Cu_{12}Sb_4S_{13}$ tetrahedrites. This work is in collaboration with my colleague Donald Morelli here at MSU.

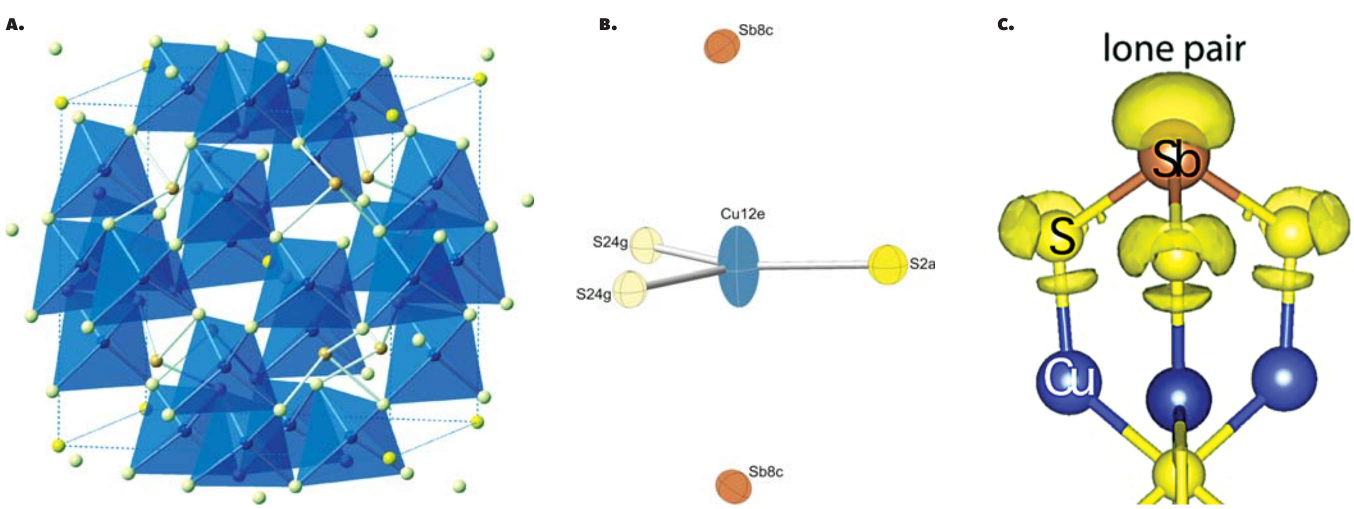


**FIGURE 3.** (A) Cu-Sb-S framework, (B) Cu guest, (C) Sb lone pairs.

## RECENT PUBLICATIONS


Yuxing Wang; Wei Lai. “Phase transition in lithium garnet oxide ionic conductors $Li_7La_3Zr_2O_{12}$: The role of Ta substitution and $H_2O/CO_2$ exposure,” *Journal of Power Sources.* 2015;275:612–620. (2015)

R. Shanmugam and W. Lai, “Study of Transport Properties and Interfacial Kinetics of $Na_{2/3}[Ni_{1/3}Mn_xTi_{2/3}]O_2$ ($x = 0, 1/3$) as Electrodes for Na-Ion Batteries,” *J. Electrochem. Soc.*, 162, A8 (2015)

Y. Wang, M. Klenk, K. Page, W. Lai, “Local Structure and Dynamics of Lithium Garnet Ionic Conductors: A Model Material $Li_5La_3Ta_2O_{12}$,” *Chem. Mater.*, 26, 5613 (2014)

R. Shanmugam and W. Lai, “$Na_{2/3}Ni_{1/3}Ti_{2/3}O_2$: “‘Bi-functional’ electrode materials for Na-ion Batteries,” *ECS Electrochem. Lett.*, 3, A23 (2014)

# Andre Lee

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■ **RESEARCH INTERESTS**

High-temperature hybrid materials, composite materials synthesis and processing, electronic packaging materials, phase transformation, x-ray synchrotron characterization

■ **LAB & LOCATION**

Inorganic-Organic Synthesis and Processing, 428 S. Shaw Lane, Room 3545

■ **SPECIAL EQUIPMENT AVAILABLE**

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

■ **GROUP MEMBERS**

PHD STUDENTS: Yang Lu, Yueline Wu, David Vogelsang.
COLLABORATING FACULTY: Prof. Robert Maleczka (Chemistry).

■ **PATENTS GRANTED**

Lee, A; Lichtenhan, J.D.; Schwab, J.J.; Phillips, S.H. Nanostructured Chemicals as Alloying Agents in Polymers. US Patent 6716919, 2004.

Lee, A.; Lichtenhan, J.D.; Liu, Q.; Fu, X.; Hait, S.; Schwab, J.J.; Blanski, R.L.; Ruth, P.N. High Use Temperature Nanocomposite Resins. US Patent 7553904, 2009.

Lee, A.; Subramanian, K.N. Composite metal matrix castings and solder compositions, and methods. US Patent 7572343, 2009.

■ **CURRENT RESEARCH FOCUS**

■ ***Applications in inorganic-organic materials.*** In 2009 an effort to develop solvent-free, processible oligoimides as matrix materials for carbon-fiber reinforced composite was initiated. The candidate inorganic-organic oligoimides based on the double-decker shaped incompletely condensed SQ architecture were explored. The inorganic nature offers service reliability at high temperatures, while organic enable processibility. The route used to obtain difunctional phenylethynylphthalimide SQ, bis-PEPI DDSQ, is shown in Figure 1. This oligoimides exhibited little or no crystallinity, a flow temperature at around 100°C and a low wetting angle to carbon fibers. In addition, the presence of the SQ cage does not retard the reaction kinetics as well as the curing of ethynyl groups to form fully cured thermosetting networks. These findings were deemed to be critical for the development of a new class of high temperature thermosetting oligoimides.

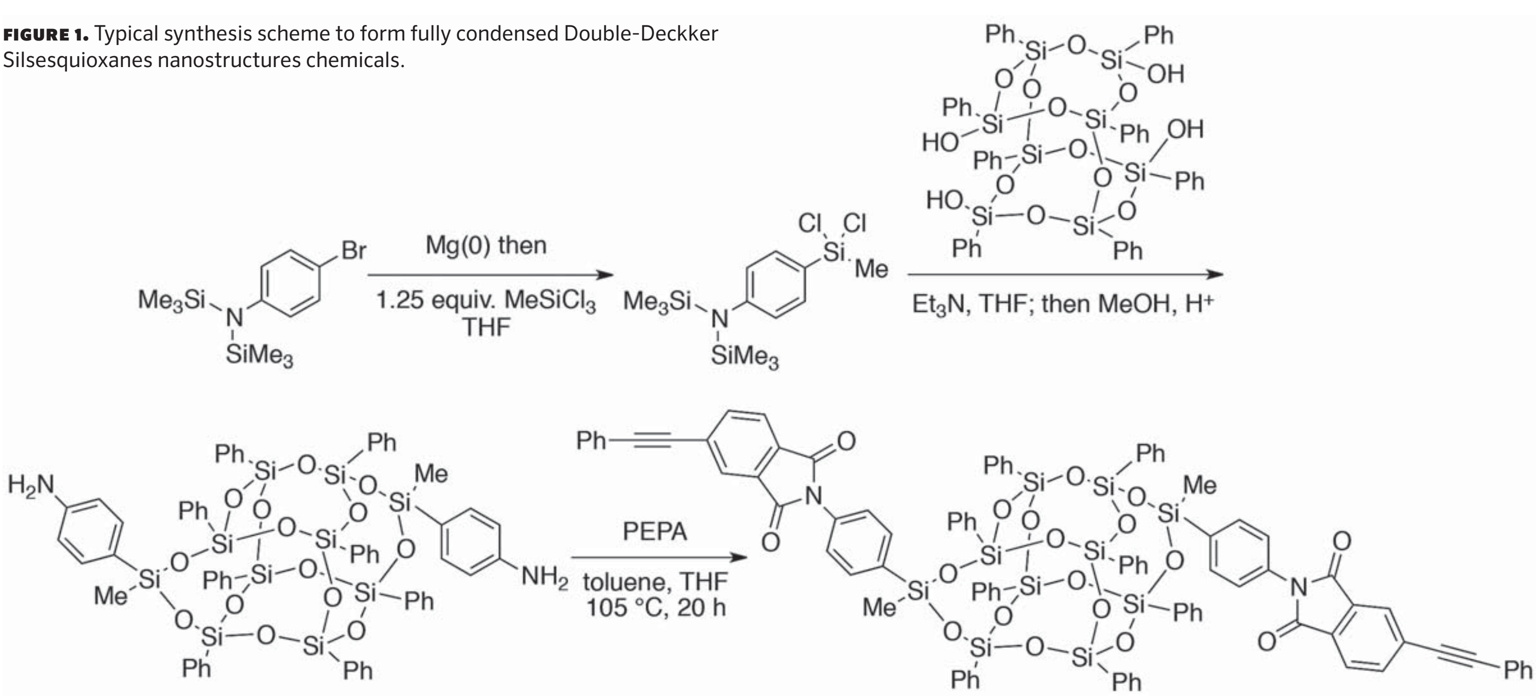
The scheme as shown in Figure 1 naturally lead to a final product can contains *trans* and *cis* isomer of the intermediate bis-amionpheny DDSQ or the final bis-PEPI DDSQ. An effort to separate the two isomers was initiated to gain better understanding on the property of these isomers and well as its mixture (Figure 2).

Taking advantage of the solubility difference of the two isomers of bis-aminophenyl DDSQ, ultra high purity of *trans* and *cis* isomers of bis-(*meta*)aminophenyl DDSQ and bis-(*para*) aminophenyl DDSQ were obtained and verified using using $^{29}$Si,$^{1}$H NMR with 2D analysis through $^{3}$J-coupled Si-H bonding.

In addition, by adjusting the ratio of THF/hexanes used, it was possible to obtain products with specified *trans/cis* ratio.

Using a mixture of *meta* and *para* aminophenyl dichlorosilane as the starting capping agents, product containing six different isomers can be obtained. Initial experiment using 50:50 mixture of *meta* and *para* aminophenyl dichlorosilane, the resultant bis-PEPI DDSQ product exhibited a viscosity that enables the process to form carbon-fiber pre-preg at temperature as low as 150°C. Moreover, the viscosity can be adjusted by controlling the ratio of the six isomers present.

**FIGURE 1.** Typical synthesis scheme to form fully condensed Double-Deckker Silsesquioxanes nanostructures chemicals.



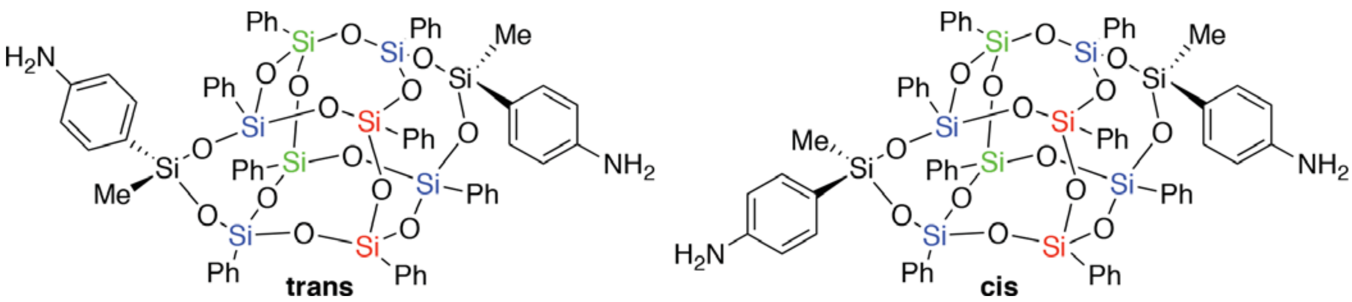


**FIGURE 2.** Chemical structures of trans and cis stereoisomers.

This product is a significant advancement in high temperature oligoimide resins. When a large-scale production is developed, it is expected to dramatically improve the performance of light-weight composites with significant reduction in the fabrication cost. Currently U.S. Air Force Research Laboratory is sponsoring the development of the large-scale production and mechanical performance database.

- ***Service reliability of Cu wire bonding packages.*** Wire bonding is a key packaging technology to make the electrical interconnections between chips and substrates. The necessity to improve density of electrical inter connects, IC density, and cost reduction warrant replacing Au with Cu in the wire bonding packages. Although fabrication processes of the fine-pitch Cu wire bonding packages has been steadily improving, the intrinsic oxidation sensitivity of Cu as compared to Au remains a significant reliability concern when Cu is bonded to environmentally active Al pads. The potential sources of reliability concern are attributed to the observed galvanic corrosion between various Cu-Al IMCs and resulting oxides. In addition, formation of less-stable, self-passivating oxides can cause interfacial cracking during the high humidity stressing that further accelerates the rate of corrosion damage. These proposed damage pathways were retarded in a recent study using Pd-coated Cu wire, where reliability was improved via controlling the diffusion and the IMC formation processes on the Cu-Al interface. Although this qualitative investigation provided a general guideline to be used for reliability improvement, electrochemical details of various entities present at Cu-Al interface are not yet fully understood. Thus accurate lifetime predication of Cu-wire bonding packages remains elusive. Moreover fundamental knowledge on the electrochemical details of Cu-Al interface will enable a systematic development of a more economical Cu wire coating or alloying solution than a solution that needs expensive Pd.

The scientific challenge of this study is to understand the stability of various oxide layers on IMCs at the Cu-X/Al interface that can provide passivation in the wire bonding package environment in molding compounds containing various corrosive chemical entities, as well as the ability of controlling the formation of these reactive interfacial IMCs in the presence of other metallic coatings or alloying. These fundamental generalizations will lead to solutions for optimized service performance and long-term service reliability of Cu-wire bonding in electronic packages. This is expected to create a fundamental pathway leading to a more economical and highly-reliable design methodology and materials selection for future electronic packages.

## RECENT PUBLICATIONS


Beth W. Schoen; Carl T. Lira; Andre Lee. “Separation and solubility of cis and trans isomers in nanostructured double-decker silsequioxanes,” *Journal of Chemical and Engineering Data*. 2014;59(5):1483–1493. (2014)

Sihan Liu; Limin Ma; Yutian Shu; K.N. Subramanian; Andre Lee; Fu Guo. “Effects of poss-silanol addition on whisker formation in Sn-based Pb-free electronic solders,” *Journal of Electronic Materials*. 2014;43(1):26–32. (2014)

B.W. Schoen; D. Holmes; A. Lee. “Identification and quantification of cis and trans isomers in aminophenyl double-decker silsesquioxanes using 1H-29Si gHMBC NMR,” *Magnetic Resonance in Chemistry*. 2013;51(8):490–496. (2013)

Yang Lu; Andre Lee; Xiufang Wen; Pihui Pi; Jiang Cheng; Zhuoru Yang. “Processing science of isotactic polypropylene fiber reinforced with halloysite nanotubes based on masterbatch dilution technique,” *Advanced Materials Research*. 2013;677:16–19. (2013)

# Ilsoon Lee

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**FIGURE 1.** Bacterial biofilm examples: body surface (teeth), ship skull, natural.

## RESEARCH INTERESTS

Polymer engineering, centered on polymer surfaces, interfaces, and self-assembly; and among these most especially polymer adhesion and thin films. My research concerns control over surface and interface properties at the molecular level, which is critically important in many existing and emerging technologies, particularly those that are based on electro-active organic and polymeric materials, and bio-active or bio-responsive materials.

## LAB

Nano Bio Engineering Laboratory (NBEL)

## GROUP MEMBERS

VISITING SCHOLAR: Dr. Joung Sook Hong (Soongshil University, Seoul, Korea). GRADUATE PHD STUDENTS: Oishi Sanyal, Jing Yu, Anna Song. UNDERGRADUATE STUDENTS: Andrew Izbick, Brooke Meharg, Chris Tawfik, Alex Hanft, Jason Thompson, Yi Ji.

## WEBSITE

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

## RECENT PATENTS GRANTED (8 TOTAL)

Lee, I.; Wang, W.; Ji, S., One-step Method for Pretreating Biomass Using Nanomixing. US Patent 8741632, June 3, 2014.

Kohli, N.; Srivastava, D.; Richardson, R.J.; Sun, J.; Lee, I.; Worden, R.M. Nanostructured Biosensor Containing Neuropathy Target Esterase Activity. US Patent 8,623,196, January 7, 2014.

Lee, I.; Hendricks, T.R. Wrinkle-free Nanomechanical Film. US Patent 8,460,785, June 11, 2013.

Worden, R.M.; Ofoli, R.Y.; Hassler, B.L.; Kohli, N.; Lee, I. Customizable and Renewable Nanostructured Interface for Bioelectronic Applications. US Patent 8,435,773, May 7, 2013.

## CURRENT RESEARCH FOCUS

The NBEL 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. Specific selective projects include:

- ***Prevention of bacterial biofilm formation on surfaces.*** Bacterial biofilms result in billions of dollars of economic loss due to contamination and corrosion of industrial equipment, biofouling of ships hulls, loss of agriculture products, and medical expenses. Furthermore, bacterial biofilm formation is responsible for millions of infections and hundreds of thousands of fatalities annually in the United States. As bacteria in biofilms are resistant to treatment with traditional antibiotics, it is critical to develop new methods to prevent and remove bacterial biofilms.
  SPONSOR: The MSU Foundation (SPG).COLLABORATOR: Dr. Chris Waters.
- ***Solar-bio-nano based wastewater system for the production of energy and potable water.*** The solar-bio-nano project for wastewater system will generate energy and produce drinking water, thus providing a potential blueprint for the future of

municipal/ agricultural wastewater treatment systems.

The integrated system will comprise three major components. First, the solar unit will use new materials and employ a novel configuration making it up to 80% lighter than traditional solar units. Second, biological conversion processes will break down wastewater and food scraps to produce methane that can be used as fuel. Finally, a nano-filtration system will then take the discharge from the biological processes to provide drinking water. In our work, we particularly focus on membrane-based purification as the tertiary treatment to treat such a typical wastewater sample that consists of food wastes and dairy effluents. We propose the use of some novel polyelectrolyte multilayer (PEM) based membranes instead of commercial reverse osmosis (RO) membranes. The idea behind using these membranes is that if we employ these membranes in the actual wastewater treatment scheme we can reduce the operating costs of the membrane-based process. So far, researches have shown that PEM membranes can be very effective for ion rejection applications. But very few researches have been done to actually test these membranes with real wastewater samples and evaluate COD reduction. These membranes were tested for two different batches of the sample and for both these batches the PEM-based membranes show much higher permeability than the RO membranes with equivalent COD reduction.

SPONSOR: DOD SERDP. COLLABORATORS: Drs. Liao (Biosystems Engineering), Engeda (ME).

- ***Affordable production of cellulose nanowhiskers/cell wall surface and interface study.*** Cellulose nanowhisker (CNW) is a renewable, recyclable, and abundant nano-sized bio-based polymer made of cellulose fibers from pulp manufacturing or biofuel production process. Superior mechanical, thermal, and biodegradable properties of CNW enable it as an ideal candidate for composite reinforcement and co-product from conventional paper making and biofuel production. It can be a promising practice to transform paper industry into biorefineries, from which a wide range of value-added products can be produced besides the traditional products. The large time investment and energy consumption become major problems for the production of CNW from different sources. Our technology has successfully combined the conventional acid hydrolysis and high shear nanomixing, synergistically promoting the separation of cellulose fibers into nano-dimension. This process is a simple and efficient one with much reduced processing time and energy input. The length of produced CNW is comparable to or shorter than those prepared from existing methods. Those CNWs uniformly disperse in an aqueous solution with a high aspect ratio of the renewable nanomaterials. 3–5 minute processing and moderate temperature condition allows the potential development of this technology to be commercialized. Existing industrial experience from microfibrillated cellulose production will be used as reference for a commercial scale-up (patent pending).

SPONSOR: MIIE & NSF. COLLABORATOR: Dr. Hodge (NSF).

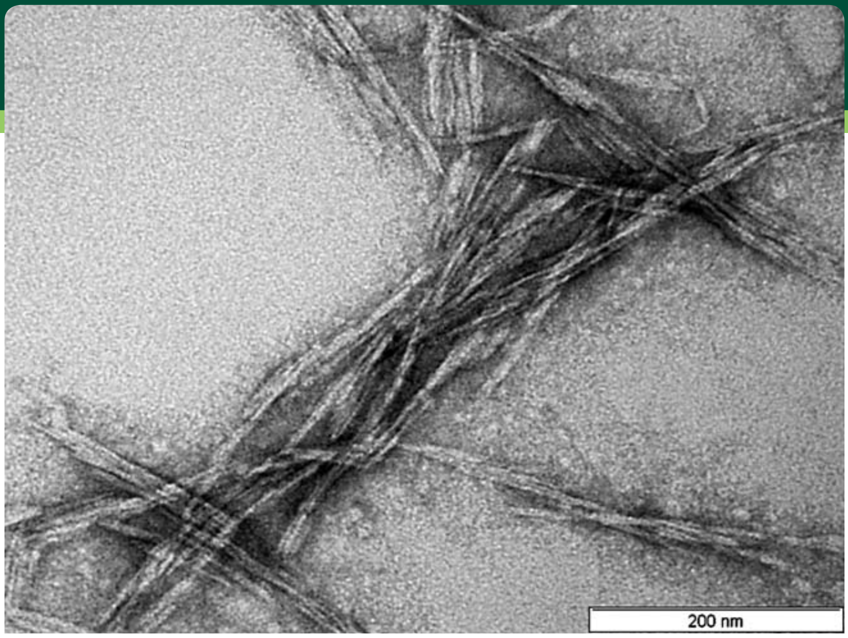


**FIGURE 2.** SEM images of CNWs extracted by acid hydrolysis at reaction temperature of 45°C.

## RECENT PUBLICATIONS

Yi Sun; Rigoberto Burgueño; Wei Wang; Ilsoon Lee. "Modeling and simulation of the quasi-static compressive behavior of Al/ Cu hybrid open-cell foams," *International Journal of Solids and Structures*. 2015;54:135–146. (2015)

Ankush A. Gokhale; Jue Lu; Rankothge R. Weerasiri; Jing Yu; Ilsoon Lee. "Amperometric Detection and Quantification of Nitrate Ions Using a Highly Sensitive Nanostructured Membrane Electrocodeposited Biosensor Array," *Electroanalysis*. 2015. (2015)

Yi Sun; Rigoberto Burgueño; Wei Wang; Ilsoon Lee. "Effect of annealing on the mechanical properties of nano-copper reinforced open-cell aluminum foams," *Materials Science and Engineering A*. 2014;613:340–351. (2014)

Shaowen Ji; Jue Lu; Zhiguo Liu; Devesh Srivastava; Anna Song; Yan Liu; Ilsoon Lee. "Dynamic encapsulation of hydrophilic nisin in hydrophobic poly (lactic acid) particles with controlled morphology by a single emulsion process," *Journal of Colloid and Interface Science*. 2014;423:85–93. (2014)

Oishi Sanyal; Ilsoon Lee. "Recent progress in the applications of layer-by-layer assembly to the preparation of nanostructured ion-rejecting water purification membranes," *Journal of Nanoscience and Nanotechnology*. 2014;14(3):2178–2189. (2014)

Ankush A. Gokhale; Ilsoon Lee. "Recent advances in the fabrication of nanostructured barrier films," *Journal of Nanoscience and Nanotechnology*. 2014;14(3):2157-–2177. (2014)

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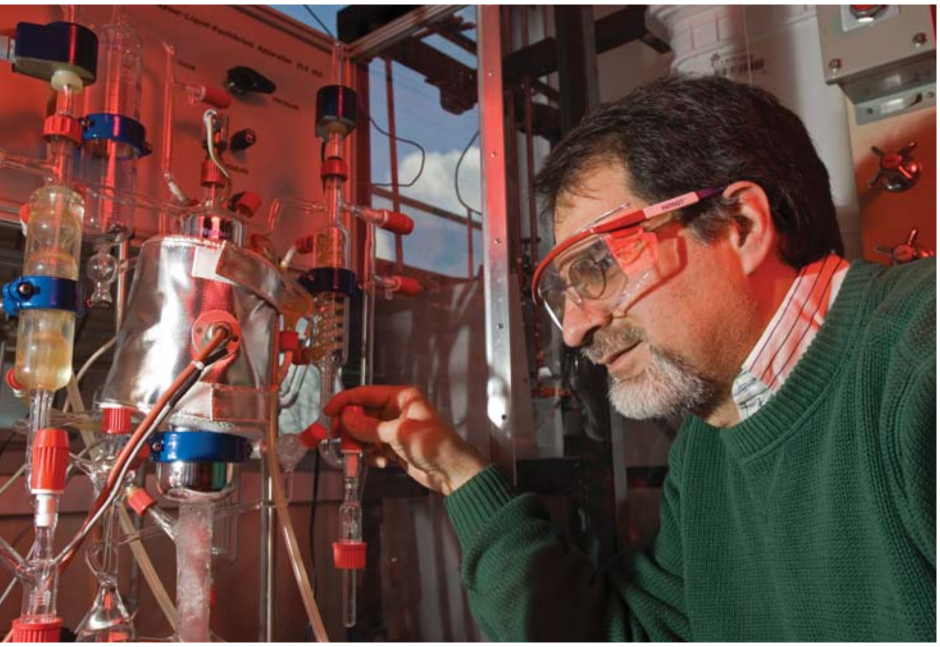
Yi Sun; Rigoberto Burgueño; Andy J. Vanderklok; Srinivasan Arjun Tekalur; Wei Wang; Ilsoon Lee. "Compressive behavior of aluminum/ copper hybrid foams under high strain rate loading," *Materials Science and Engineering A*. 2014;592:111–120. (2014)

# Carl Lira

**Associate Professor | lira@egr.msu.edu | 517.355.9731 | 428 S. Shaw Lane, Room 2261**



### RESEARCH INTERESTS

Properties of bio-derived chemicals and fuels

### LABS & LOCATIONS

Properties Lab, 418 S. Shaw Lane, Room 2255.
Reactive Distillation Pilot Facility, 3900 Collins Rd.

### WEBSITES

http://researchgroups.msu.edu/liragroup
http://researchgroups.msu.edu/reactivedist

### SPECIAL EQUIPMENT AVAILABLE

Vapor-liquid equilibria measurements, flash point, cloud point, densitometry, low- and high-pressure speed of sound

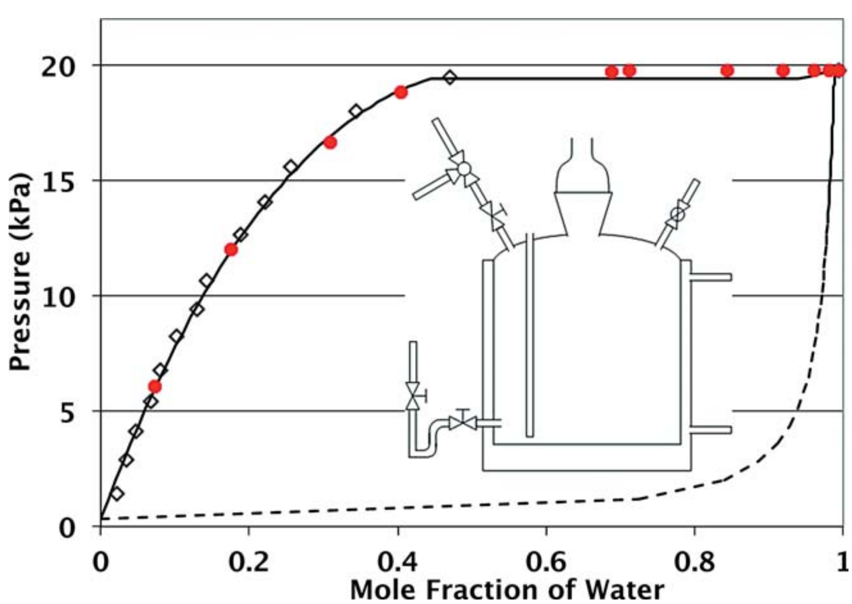



**FIGURE 1.** P-x diagram of ethyl levulinate + water at 60°C compared with the NRTL-HOC model.

### GROUP MEMBERS

Ann L. Lown, Aseel Bala-Ahmed, Dr. Lars Peereboom

### RECENT PATENTS GRANTED (8 TOTAL)

Miller, D.J.; Hong, X.; Lira, C.T.; McGiveron, O. Methods for Making 1,3-Dihydroxyacetone (DHA) from Glycerol. US Patent 8,735,633 B2, May 27, 2014.

Asthana, N.S.; Miller, D.J.; Lira, C.T.; Bittner, E. Process for Producing Mixed Esters of Fatty Acids as Biofuels. US Patent 8,613,780, December 24, 2013.

### CURRENT RESEARCH FOCUS

Make it, boil it, dissolve it, purify it. The Lira Research group is fascinated by characterizing these relatively common properties for pure components and mixtures, and the way the chemical structure determines these properties. When an alternative fuel is developed and blended with petroleum fuel, what are the cold flow properties? What is the effect on the boiling curve? When new chemicals are made from renewable feedstocks, how will they behave in a reactive distillation column? We are also interested in improving modeling of vapor-liquid-liquid equilibria that occurs frequently for bioderived molecules.

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

  Our phase equilibria measurements support the MSU reactive distillation facility and were vital in development of our process development for diethyl succinate by reactive distillation. We have filed a patent on a process to react the sodium succinate salt directly from the fermentation product to diethyl succinate intermediates, bypassing isolation of succinic acid.

  An example of P-x measurements are shown in Figure 1, for ethyl levulinate + water.

  RECENT SPONSORS: DOE, DLA, misc industry.

  COLLABORATORS: Dennis Miller

- ***Alternative fuel properties.*** This work models properties of alternative fuels and their blends with petroleum-derived fuels. Differing fuel properties can create compatibility issues in the field. We are developing methods to quickly characterize the behavior of blends and provide predictive tools for blend cloud point, distillation curve, average molecular weight and cetane number. Surrogates with a finite number of components are used to represent the paraffin, isoparaffin, aromatic, and naphthene distribution in the fuels. Alternative fuels have composition profiles significantly different than petroleum fuels. Figure 2 shows the distillation curve behavior of traditional JP-8 fuel and several alternative fuels.

  SPONSORS: U.S. Army, Tank Automotive Research Development and Engineering Center. COLLABORATORS: Eric Sattler (USA), Nicole Hubble (USA), Linda Schafer (USAF).

- ***Improved association-based models for separations in the bioeconomy.*** With industrial focus moving to bioderived feedstocks, the need for improved process modeling is acute; conventional models with adjustable parameters do not correlate data accurately enough for extrapolations in temperature or to new compositions. Thus, precise process design for streams with these components requires many experimental measurements and expensive, slow pilot-plant studies. Improved models will greatly enhance the efficiency of renewables-based process development. This project is developing improved models that include meaningful representation of hydrogen bonding of oxygen-containing molecules. Popular predictive and correlative models (UNIFAC, NRTL) do not use the correct functional form to represent hydrogen bonding. This work strives to integrate association approaches such as Wertheim's theory together with meaningful spectroscopic measurements and quantum chemical calculations to improve modeling of hydrogen-bonding system. Figure 3 shows an early version of the modeling capabilities

  COLLABORATORS: James (Ned) Jackson (Chemistry), N. Patel (Dow Chemical), P. Mathias (Fluor), T. Frank and D. Vu (Dow Chemical), E. Cheluget and C. Rhodes (Honeywell).

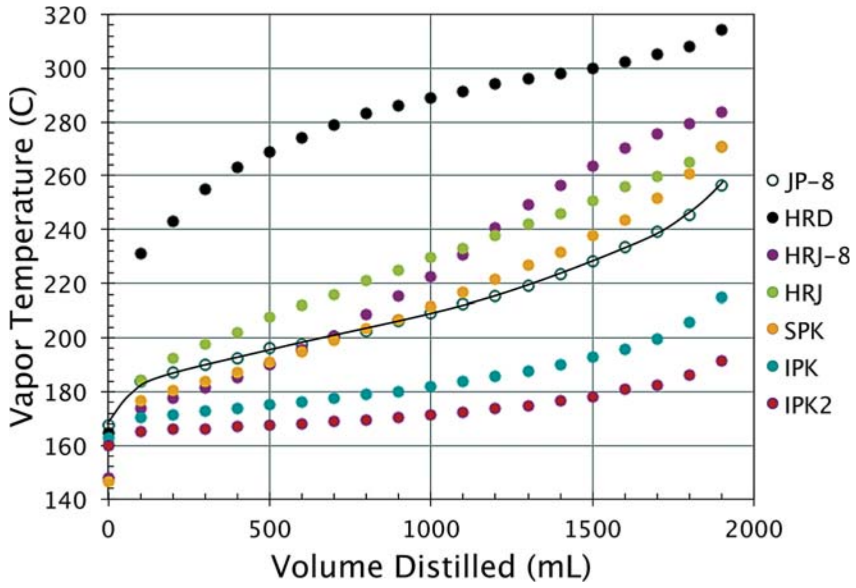



**FIGURE 2.** Fuel volatility is related to both ease of starting. Note the wide distribution of boiling behavior exhibited by the fuels.

### RECENT PUBLICATIONS

Beth W. Schoen; Carl T. Lira; Andre Lee. "Separation and solubility of cis and trans isomers in nanostructured double-decker silsequioxanes," *Journal of Chemical and Engineering Data*. 2014;59(5):1483–1493. (2014)

Alexander J. Resk; Lars Peereboom; Aspi K. Kolah; Dennis J. Miller; Carl T. Lira. "Phase equilibria in systems with levulinic acid and ethyl levulinate," *Journal of Chemical and Engineering Data*. 2014;59(4):1062–1068. (2014)

Anne L. Lown; Lars Peereboom; Sherry A. Mueller; James E. Anderson; Dennis J. Miller; Carl T. Lira. "Cold flow properties for blends of biofuels with diesel and jet fuels," *Fuel*. 2014;117(PART A):544–551. (2014)

Mark Urban-Lurain; Melanie M. Cooper; Kevin C Haudek; Jennifer Julia Kaplan; Jennifer K. Knight; Paula P. Lemons; Carl T. Lira; John E. Merrill; Ross Nehm; Luanna B. Prevost; et al. "Expanding a national network for automated analysis of constructed response assessments to reveal student thinking in STEM," ASEE Annual Conference and Exposition, Conference Proceedings. 2014. (2014)

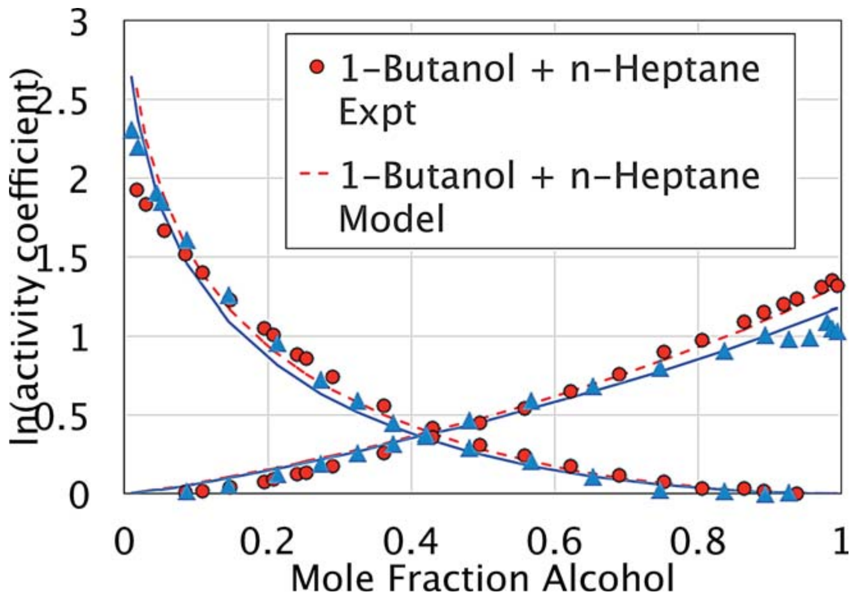



**FIGURE 3.** After representing the hydrogen bonding in pure alcohols, the predictions of solution nonidealities in mixtures with hydrocarbons are well captured without using any adjustable mixture parameters.

# Richard Lunt

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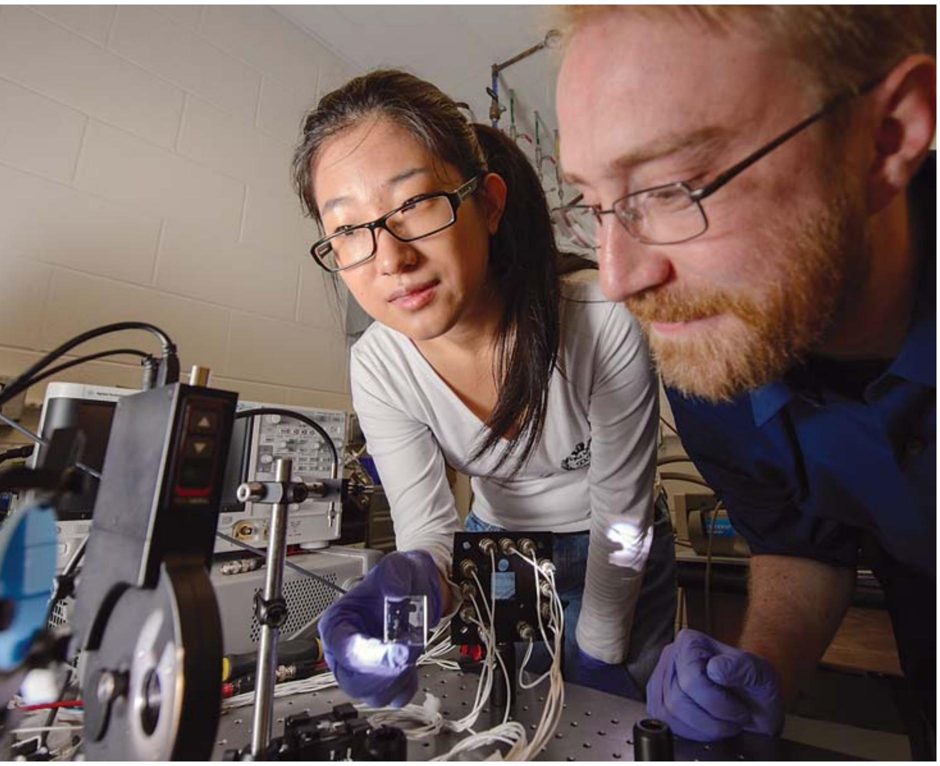

**RESEARCH INTERESTS**

Organic and molecular electronics, renewable energy and utilization, solar cells, light-emitting diodes, excitonic photophysics, crystal growth

**LAB**

Molecular and Organic Excitonics Laboratory

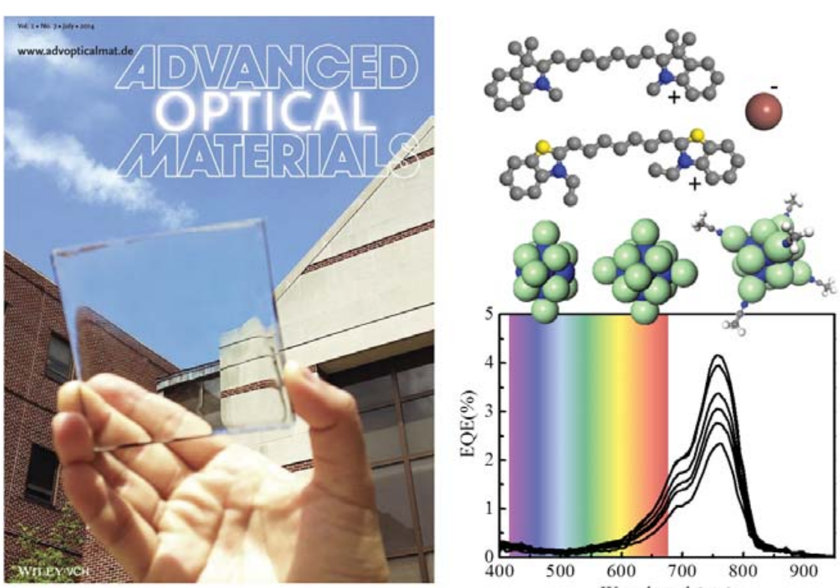


**FIGURE 1.** LEFT: Highlight of our work on the cover of *Adv Optical Materials* showing a photograph of the pioneering transparent luminescent solar concentrator (LSC) system that selectively harvests infrared light. RIGHT: Diagram of excitonic molecules for these transparent concentrators (*top*) and the demonstrated quantum efficiency in the infrared (*bottom*).

**WEBSITE**

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

**SPECIAL EQUIPMENT AVAILABLE**

Thin film device fabrication, patterning, and testing; in situ diffraction; ellipsometry; luminescence spectroscopy

**GROUP MEMBERS**

VISITING RESEARCHERS: Dr. Richa Pandy; Dr. Miles Barr (Ubiquitous Energy). POSTDOCS: Dhanashree Moghe, Jorge Rossero, Lily Wang. GRADUATE STUDENTS: Pei Chen, Joe Hagerty, Padmanaban (Paddy) Kuttipillai, Chris Traverse, Margaret (Peggy) Young, Yimu Zhao. UNDERGRADUATE STUDENTS: Kevin Chase, Natalia Chamorro, Juan Mena Lapaix, Lucas Layher, Tyler Patrick, John Suddard, Brian Wingate.

**RECENT PATENTS GRANTED** (8 TOTAL)

Forrest, S.R.; Lunt, R. Ordered organic-organic multilayer growth. US Patent 8933436, January 13, 2015.

Forrest, S.R.; Lunt, R. Growth of ordered crystalline organic films. US Patent 8912036, December 16, 2014.

Forrest, S.R.; Slootsky, M.; Lunt, R. Concave-hemisphere-patterned organic top-light emitting device. US Patent 8633497, January 21, 2014.

Forrest, S.R.; Yang, F.; Lunt, R. Apparatus and method for deposition for organic thin films. US Patent 8440021, May 14, 2013.

**CURRENT RESEARCH FOCUS**

The Molecular and Organic Excitonics laboratory focuses on inorganic and organic excitonic materials for (1) low-cost solar energy production and (2) efficient energy utilization. We look to exploit oriented, crystalline, nanostructured, and excitonic films through organic-inorganic and organic-organic interactions while studying fundamental relationships between structure and photophysical properties. Ultimately we aim to apply this understanding to enhance device efficiencies, lifetime, and create new 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.

- ***Excitonics for building integrated transparent PVs and solar concentrators.*** We have been developing an additive, transparent, molecular photovoltaic that can retain a high degree of visible transparency, while absorbing ultraviolet 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.

- ***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.

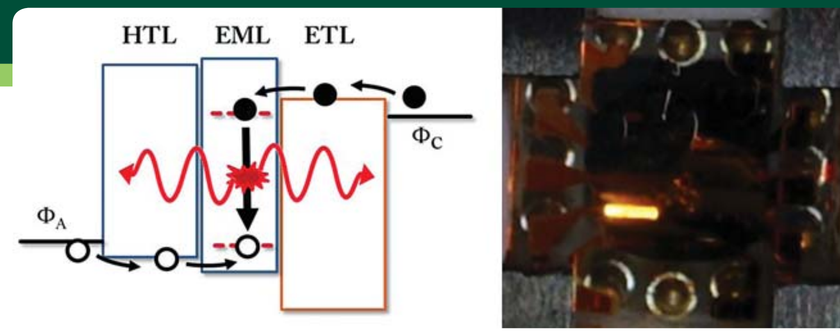


**FIGURE 2.** LEFT: Schematic energy-level diagram. RIGHT: Operation of a phosphorescent light-emitting diode.

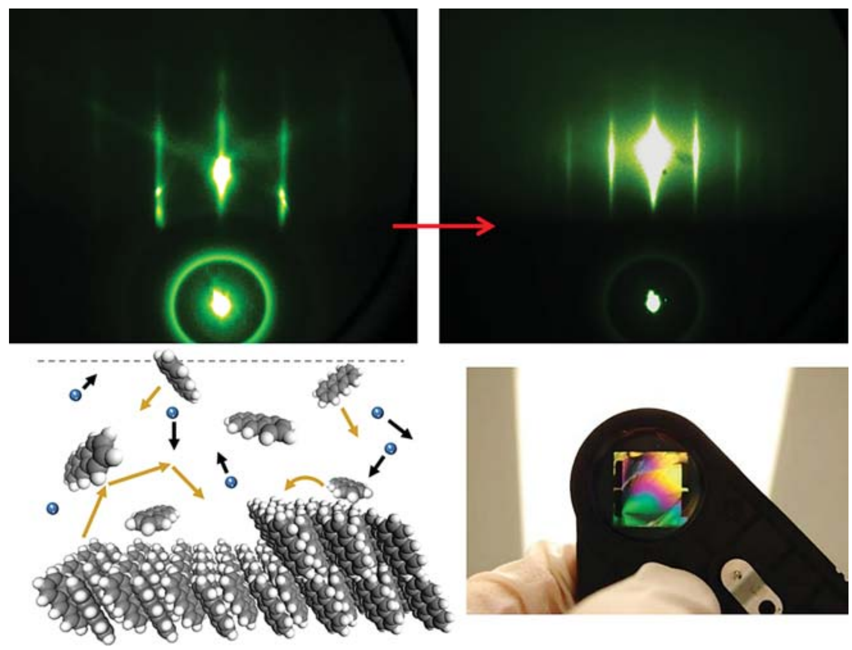

**FIGURE 3.** TOP: In situ grazing-incidence electron diffraction patterns of heteroepitaxial organic crystal growth. BOTTOM, LEFT: Schematic of molecular crystal growth dynamics. BOTTOM, RIGHT: Large area organic crystal films between two polarizers.

## RECENT PUBLICATIONS

Y. Ding; M. Young; Y. Zhao; C. Traverse; A. Bernard; R. Lunt. "Influence of Photovoltaic Angle-Dependence on Overall Power Output for Fixed Building Integrated Configurations," *Solar Energy Materials and Solar Cells*. 132.523–527. (2015)

Yimu Zhao; Garrett A. Meek; Benjamin G. Levine; Richard R. Lunt. "Near-infrared harvesting transparent luminescent solar concentrators," *Advanced Optical Materials.* 2014;2(7):606–611. (2014)

Christopher J. Traverse; Margaret Young; Sean Wagner; Pengpeng Zhang; Per Askeland; Miles C. Barr; Richard R. Lunt. "Efficient zinc sulfide cathode layers for organic photovoltaic applications via n-type doping," *Journal of Applied Physics*. 2014;115(19). (2014)

Patrick R. Brown; Donghun Kim; Richard R. Lunt; Ni Zhao; Moungi G. Bawendi; Jeffrey C. Grossman; Vladimir Bulović. "Energy level modification in lead sulfide quantum dot thin films through ligand exchange," *ACS Nano*. 2014;8(6):5863–5872. (2014)

C. Jiang; R.R. Lunt; P.M. Duxbury; P.P. Zhang. "High-performance inverted solar cells with a controlled ZnO buffer layer," *RSC Advances*. 2014;4(7):3604–3610. (2014)

R. R. Lunt; R. J. Holmes. "Small-Molecule and Vapor-Deposited Organic Photovoltaics," in *Organic Solar Cells: Fundamentals, Devices, and Upscaling*. Edited by B. R. Rand and H. Richter. (2014)

M. Young; C. J. Traverse; R. Pandey; M. C. Barr; R. R. Lunt. "Angle Dependence of Transparent Photovoltaics in Conventional and Inverted Configurations," *Appl. Phys. Lett.*, 103, 133304, 2013.

Y. Zhao; R. R. Lunt. "Transparent Luminescent Solar Concentrators for Large-Area Solar Windows," *Adv. Energy Mat.* 3, 1143–1148, (2013)

# Dennis Miller

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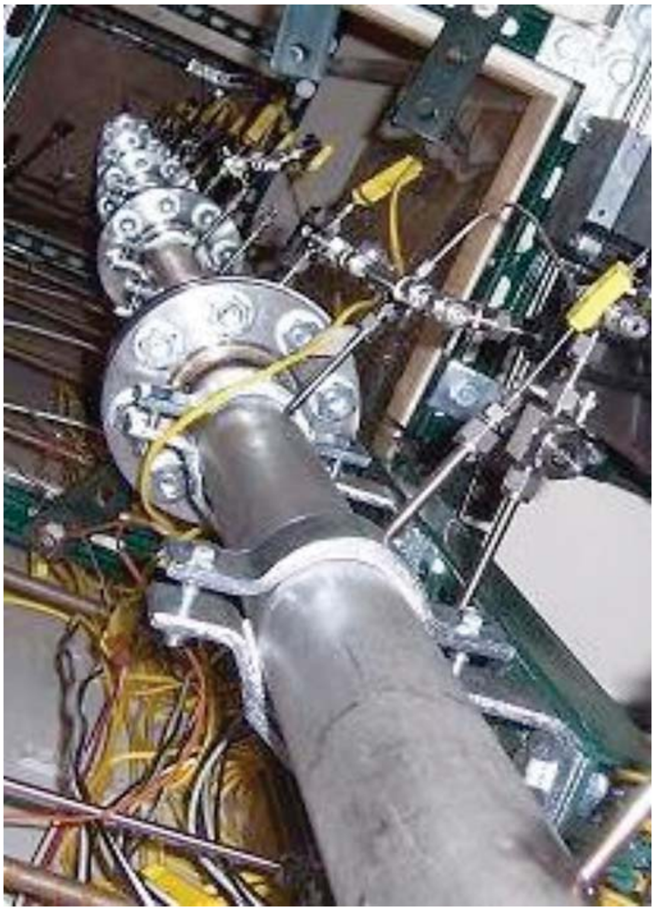


**RESEARCH INTERESTS**

Catalysis, chemicals from biomass, reactive separations

**LAB LOCATIONS**

428 S. Shaw Lane, Rooms 2535 & 2575; MBI Pilot Plant

**WEBSITE**

http://www.chems.msu.edu/people/profile/millerd
http://www.chems.msu.edu/php/resproj.php?user=millerd

**SPECIAL EQUIPMENT AVAILABLE**

We have a pilot-scale reactive separations facility located at the MBI Building on campus. We have laboratory- and pilot-scale capabilities in catalysis, and a full slate of catalyst characterization instruments.

**GROUP MEMBERS**

RESEARCH STAFF: Lars Peereboom; RESEARCH FACULTY: Aspi Kolah; GRADUATE STUDENTS: Aaron Oberg, Arati Santhanakrishnan, Iman Nezam, Tyler Jordison

**RECENT PATENTS GRANTED** (23 TOTAL)

Asthana, N.; Miller, D.J.; Lira, C.T.; Bittner, E. Process for Producing Mixed Esters of Fatty Acids as Biofuels. US Patent 8,894,725, November 25, 2014.

Hong, X.; Lira, C.T.; McGiveron, O.; Miller, D.J. Methods for Making 1,3-Dihydroxyacetone from Glycerol. US Patent 8,735,633, May 27, 2014.

Asthana, N.; Miller, D.J.; Lira, C.T.; Bittner, E. Process for Producing Mixed Esters of Fatty Acids as Biofuels. US Patent 8,613,780, December 24, 2013.

Orjuela, A., Yanez-McKay, A.; Lira, C.T., Miller, D.J. An Improved Process for Organic Acid Recovery from Fermentation Solutions. US Patent 8,293,935, October 23, 2012.

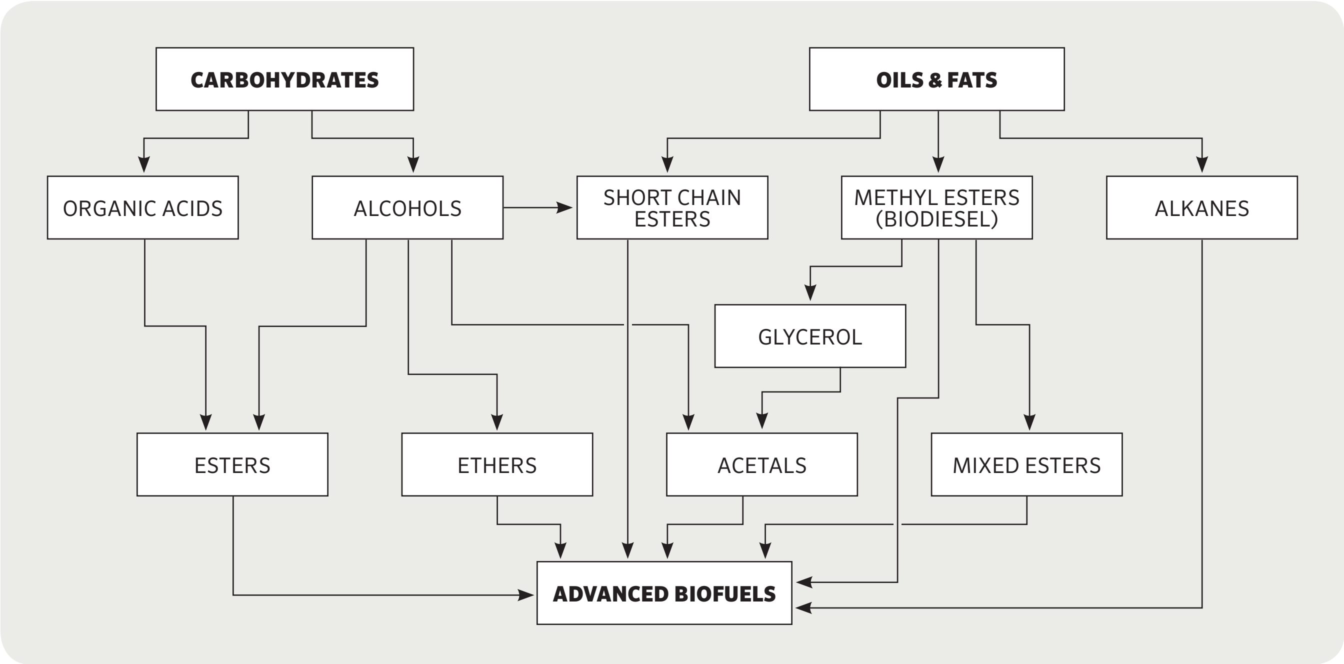
**CURRENT RESEARCH FOCUS**

The supplementing of America's abundant fossil resources with fuels and chemicals derived from biomass remains important for generation of economic opportunities and for fostering national energy independence. In the laboratories of the Miller group, cutting edge technology in heterogeneous catalysis and advanced processing is implemented to effectively convert biomass and biomass-derived intermediates to chemical products and fuels that compete with petroleum-based products in the current socio-economic environment.

The Miller group has examined a number of chemical systems directed at energy and materials production from renewable feedstocks. These have included the catalytic upgrading of biomass platform intermediates, mainly produced in fermentation processes, with the goal of building technical capabilities for the emerging biorefinery. In most cases, the overarching goal of the catalytic chemistry is deoxygenation of the biomass intermediate to a product that replaces a petroleum-derived counterpart. Classes of platform intermediates include carboxylic acids, sugar alcohols, linear alcohols, furanic compounds, and other derivatives; because these platform intermediates are typically of low volatility and are less thermally stable than their petroleum analogs, we have developed expertise in carrying out catalysis at mild temperatures under elevated hydrogen pressures in aqueous solution. The ability to design and prepare catalysts, characterize reaction pathways, and monitor chemical reaction kinetics have led to significant interactions with industrial partners, national laboratories, and agricultural groups.

The Miller group has partnered with the MSU engine group in mechanical engineering to produce and test advanced biofuels for internal combustion engines. Moving past today's first-generation ethanol and biodiesel, emphasis has been placed on developing advanced biofuels with enhanced engine performance, high energy density, and storage and flow properties that facilitate their use as direct replacements for petroleum-derived fuels.

The Miller group uses reactive separations as a platform technology for process intensification. The group operates the MSU Reactive Distillation Facility, a full pilot-scale system consisting of two ten-meter reactive distillation columns located at MBI on the MSU campus. One column is glass for atmospheric pressure and vacuum operation; the second is stainless steel for elevated pressure studies. Reactive distillation is well suited for reaction systems that are limited by chemical equilibrium, as the removal of one product by distillation allows the reaction to be driven to completion within the column. Current work emphasizes enhanced process intensification in reactive separation processes, including experimental and modeling studies of side reactors and energy integration.




## RECENT PUBLICATIONS


Chun Ho Lam; Christy B. Lowe; Zhenglong Li; Kelsey N. Longe; Jordan T. Rayburn; Michael A. Caldwell; Carly E. Houdek; Jack B. Maguire; Christopher M. Saffron; Dennis J. Miller; et al. "Electrocatalytic upgrading of model lignin monomers with earth abundant metal electrodes," *Green Chemistry*. 2015;17(1):601–609. (2015)

Alexander J. Resk; Lars Peereboom; Aspi K. Kolah; Dennis J. Miller; Carl T. Lira. "Phase equilibria in systems with levulinic acid and ethyl levulinate," *Journal of Chemical and Engineering Data*. 2014;59(4):1062–1068. (2014)

Shantanu Kelkar; Christopher M. Saffron; Zhenglong Li; Seong-Su Kim; Thomas J. Pinnavaia; Dennis J. Miller; Robert Kriegel. "Aromatics from biomass pyrolysis vapour using a bifunctional mesoporous catalyst," *Green Chemistry*. 2014;16(2):803–812. (2014)

Zhenglong Li; Shantanu Kelkar; Lauren Raycraft; Mahlet Garedew; James E. Jackson; Dennis J. Miller; Christopher M. Saffron. "A mild approach for bio-oil stabilization and upgrading: Electrocatalytic hydrogenation using ruthenium supported on activated carbon cloth," *Green Chemistry*. 2014;16(2):844–852. (2014)

Maria Enquist-Newman; Ann Marie E. Faust; Daniel D. Bravo; Christine Nicole S. Santos; Ryan M. Raisner; Arthur Hanel; Preethi Sarvabhowman; Chi Le; Drew D. Regitsky; Susan R. Cooper; et al. "Efficient ethanol production from brown macroalgae sugars by a synthetic yeast platform," *Nature*. 2014;505(7482):239–243. (2014)

Anne L. Lown; Lars Peereboom; Sherry A. Mueller; James E. Anderson; Dennis J. Miller; Carl T. Lira. "Cold flow properties for blends of biofuels with diesel and jet fuels," *Fuel*. 2014;117(PART A):544–551. (2014)

# Donald Morelli

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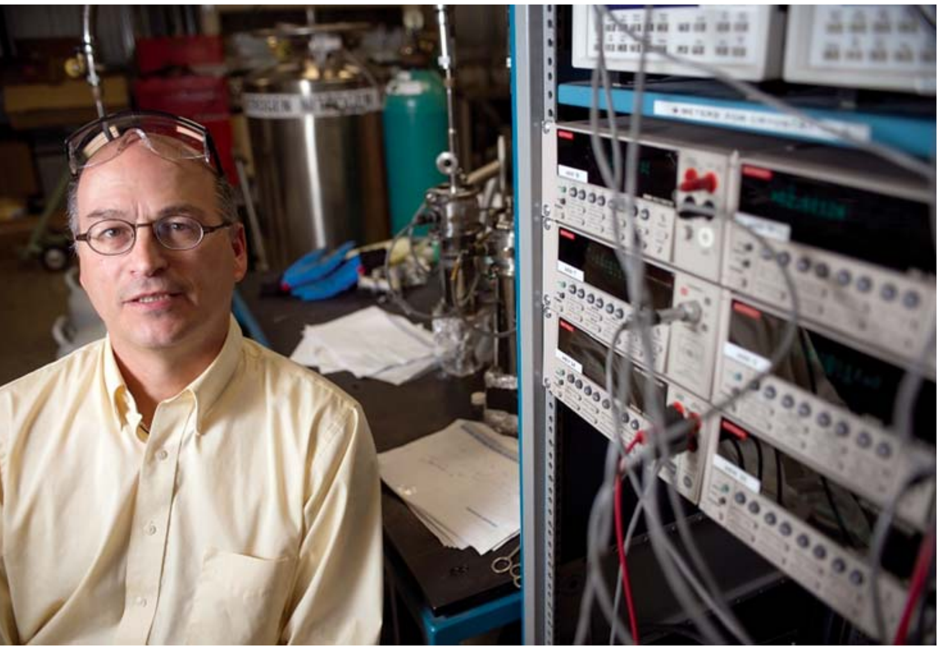

**RESEARCH INTERESTS**

Materials physics; new semiconductors for energy applications; thermal and electronic transport in solids

**LAB & LOCATION**

Electronic Materials Laboratory, E172 Engineering Research Complex

**WEBSITE**

http://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

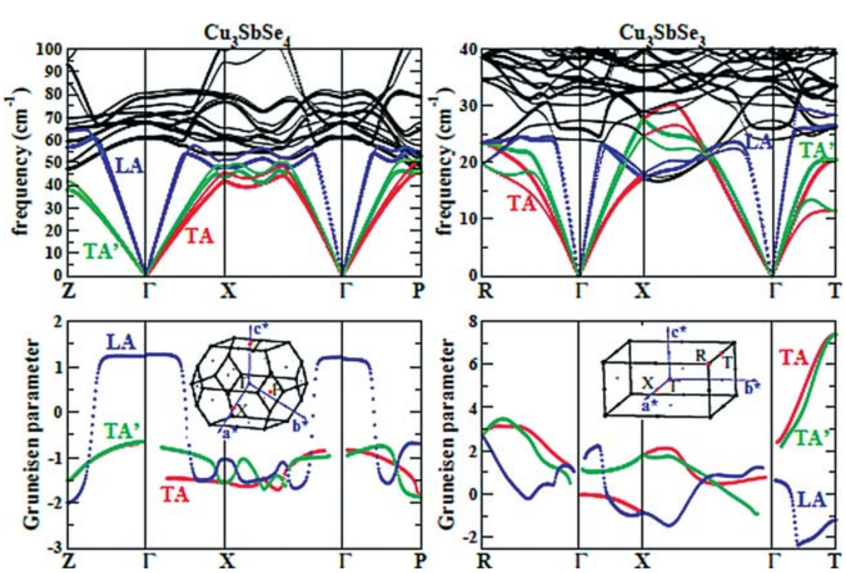


**FIGURE 1.** Calculation of the lattice dynamics of $Cu_3SbSe_4$ and $Cu_3SbSe_3$. The large Grüneisen parameters shown in the bottom panel for $Cu_3SbSe_3$ indicates that this compound will exhibit very low thermal conductivity.

**GROUP MEMBERS**

Vijay Ponnambalam, Gloria Lehr, Xu Lu, Winston Carr, Jared Williams, Spencer Waldrop, Daniel Weller

**RECENT PATENTS GRANTED** (23 TOTAL)

Kadle, P.S.; Wolfe IV, E.; Heremans, J.P.; Morelli, D.T. Thermoelectrically heated/cooled seat with improved transient response using a proportioning valve. US Patent 7610767, November 3, 2009.

Kadle, P.S.; Wolfe IV, E.; Heremans, J.P.; Morelli, D.T. Thermally conditioned container for a vehicle. US Patent 7533535, May 19, 2009.

Heremans, J.P.; Thrush, C.M.; Morelli, D.T. Thermoelectric materials comprising nanoscale inclusions to enhance seebeck coefficient. US Patent 7365265, April 29, 2008.

Oberdier, L.M.; Schroeder, T.; Disser, R.J.; Dewar, T.M.; Baudendistel, T.A.; Lequesne, B.; Morelli, D.T. Robust detection of strain with temperature correction. US Patent 7362096, April 22, 2008.

**CURRENT RESEARCH FOCUS**

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 U.S. 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:

- ***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 employed state of the art computational approaches to study the lattice dynamics of a class of promising semiconductors (Figure 1). We

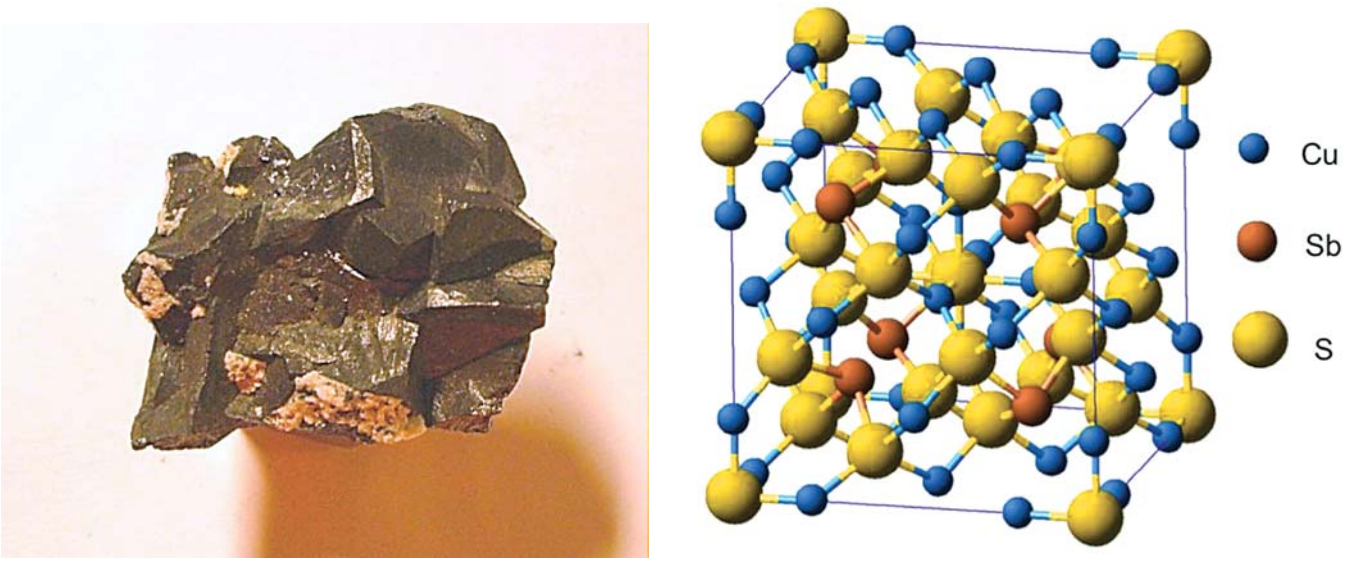


**FIGURE 2.** A natural mineral tetrahedrite polycrystal (*left*). This compound is the most widespread sulfosalt on earth; it is also a semiconductor whose properties can be tailored to produce high thermoelectric figure of merit. The crystal structure of this compound is shown on the right.

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 $Cu_{12}Sb_4S_{13}$, 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 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 $YbAl_2$ and $YbCu_2Si_2$. 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.

## RECENT PUBLICATIONS


Winston D. Carr; Donald T. Morelli. "Influence of doping and solid solution formation on the thermoelectric properties of chalcopyrite semiconductors," *Journal of Alloys and Compounds*. 2015;630:277–281. (2015)

Derak James; Xu Lu; Alexander Chi Nguyen; Donald Morelli; Stephanie L. Brock. "Design of lead telluride based thermoelectric materials through incorporation of lead sulfide inclusions or ligand stripping of nanosized building block," *Journal of Physical Chemistry C*. 2015;119(9):4635–4644. (2015)

V. Ponnambalam; Donald T. Morelli. "Thermoelectric Investigation of the Pseudo Binary System PbTe–CoSe2," *Journal of Electronic Materials*. 2015. (2015)

Xu Lu; Donald T. Morelli; Yi Xia; Vidvuds Ozolins. "Increasing the thermoelectric figure of merit of tetrahedrites by Co-doping with nickel and zinc," *Chemistry of Materials*. 2015;27(2):408-–413. (2015)

Gloria J. Lehr; Donald T. Morelli; Hyungyu Jin; Joseph P. Heremans. "$YbCu_2Si_2$–$LaCu_2Si_2$ Solid Solutions with Enhanced Thermoelectric Power Factors," *Journal of Electronic Materials*. 2014. (2014)

Hui Sun; Xu Lu; Hang Chi; Donald T. Morelli; Ctirad Uher. "Highly efficient $(In_2Te_3)_x(GeTe)_{3-3x}$ thermoelectric materials: A substitute for TAGS," *Physical Chemistry Chemical Physics*. 2014;16(29):15570–15575. (2014)

Yongsheng Zhang; Vidvuds Ozoliniņš; Donald Morelli; C. Wolverton. "Prediction of new stable compounds and promising thermoelectrics in the Cu-Sb-Se system," *Chemistry of Materials*. 2014;26(11):3427–3435. (2014)

E. Lara-Curzio; A.F. May; O. Delaire; M.A. McGuire; X. Lu; Cheng-Yun Liu; E.D. Case; D.T. Morelli. "Low-temperature heat capacity and localized vibrational modes in natural and synthetic tetrahedrites," *Journal of Applied Physics*. 2014;115(19). (2014)

V. Ponnambalam; Donald T. Morelli. "Thermoelectric properties of light-element-containing zintl compounds $CaZn_{2-x}Cu_xP_2$ and $CaMnZn_{1-}Cu_xP_2$ ($x$ = 0.0–0.2)," *Journal of Electronic Materials*. 2014;43(6):1875–1880. (2014)

Xu Lu; Donald Morelli "The effect of Te substitution for Sb on thermoelectric properties of tetrahedrite," *Journal of Electronic Materials*. 2014;43(6):1983–1987. (2014)

# Ramani Narayan

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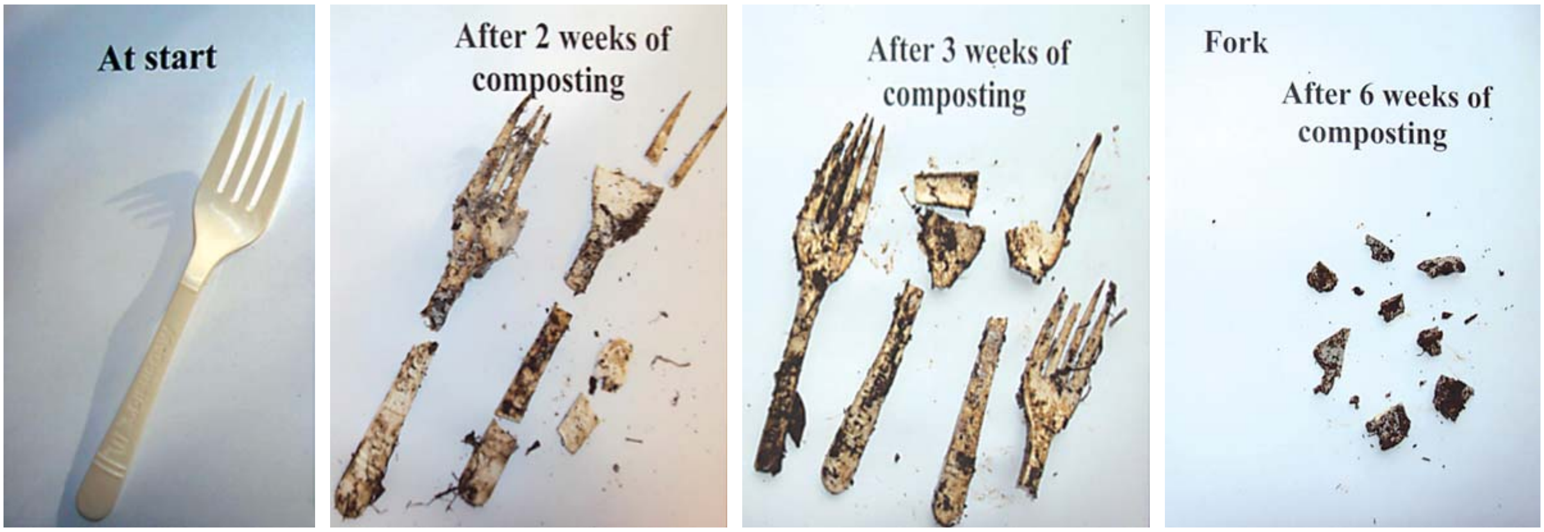



**FIGURE 1.** Biodegradability of new PLA-based forks in a composting environment.


## RESEARCH INTERESTS

Design and engineer BioPlastics, specifically biobased materials; 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 LOCATION

MBI, 3815 Technology Blvd., Lansing, MI

## WEBSITE

http://www.msu.edu/~narayan

## GROUP MEMBERS

SENIOR STAFF RESEARCHERS: Dr. Daniel Graiver (Adjunct Prof, MSU), Ken Farminer (formerly with Dow Corning). POSTDOCTORAL & VISITING RESEARCH FELLOWS: Dr. Mohan Patil (UICT, India), Dr. Elodie Hablot (Univ. of Strasbourg, France), Dr. Yuya Tachibana (AIST, Japan), Professor Philippe Dubois (Univ of Mons, Belgium), Professor Y. Z. Wang (Sichuan University, China), Dr. Jean Marie (Ben) Raquez (Univ of Mons, Belgium). GRADUATE STUDENTS: Chetan Tambe, Jeff Schneider, Yanjie Zhao, Atishi Bali, Samaneh Rahimi, Hugh McDonald, Sayli Bote, Preetam Giri. UNDERGRADUATE STUDENTS: Brandon Duquette, Caleb Andrews, Natasha Baig, Ariel Rose, Kaitlyn Borque, Kylash Sivakumar, John Kaufmann.

## RECENT PATENTS GRANTED (28 TOTAL)

Narayan, R.; Graiver, D.; Farminer, K.W. Bio-based oxygenated esters and diesters and method of preparation thereof. US Patent 8349032, January 8, 2013.

Narayan, R; Graiver, D.; Dewasthale, S.; Hablot, E. Interpenetrating polymer networks derived from silylated triglyceride oils and polysiloxanes. US Patent 900100, April 7, 2015.

Narayan, R.; Graiver, D.; Farminer, K.W.; Srinivasan, M. Moisture curable oil and fat compositions and processes for preparing the same. US Patent 8110036, February 7, 2012.

## CURRENT RESEARCH FOCUS

Biobased Materials (Narayan) 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, arts and crafts and toy materials, and biomedical applications. The group's biobased materials technology platform is covered by 29 patents and 150 peer-reviewed publications, and eight technologies have been licensed or resulted in a spin-out company. 15 Ph.D and 18 M.S. degree students have graduated from the group. Currently there are eight graduate students, five undergraduate students, two senior research staff, one postdoctoral and several visiting research fellows in the group.

Funded by a Phase I & II NSF STTR project with KTM Industries (www.ktmindustries.com) a local Michigan small business, we designed and engineered a portfolio of biodegradable starch based biofoam materials for the protective packaging and insulation market. These materials have (A) the performance of current petro/fossil based polyethylene and polystyrene foam materials, (B) 100% biobased carbon content, and (C) can be safely, completely, and efficiently biodegraded in soil or composting operations at the end-of-life.

Our technology on biobased and biodegradable-compostable polymers using biopolyesters and poly(lactic acid) (PLA) has been commercialized through Northern Technologies International (www.ntic.com), a $150+ million publicly traded micro-cap company formed a strategic partnership with BioPlastic Polymers to commercialize the bioplastics technology world-wide under the brand name Natur-Tec (www.natur-tec.com). We published two papers based on silicone polymers focusing on biobased and compostable PLA polymers. Our work on the crystallization behavior and kinetics of PLA polymers, and the rheological modification of PLA, is part of a NSF-STTR Phase II project with Northern Technologies. Another major focus is on engineering a process for the thermal recycling of PLA to lactide monomer.

In cooperation with NTIC, we are working on a Department of Defense (DOD) Phase II SBIR project on developing non-plastic biobased and biodegradable coatings for non-plastic bags for the Navy. These bags are designed to have high strength, light weight, water resistance, and can be readily treated with other organic wastes in the on-board waste processing equipment. When discharged into the ocean they are readily marine biodegradable as defined by ASTM D7081 specification standards. The coatings technology involves grafting reactive silanes onto the double bonds of the soybean oil (plant oils) and subjecting it to moisture cure. The technology has been scaled to run at an industrial converter and prototype bags have been made.

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 soybeans (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 soymeal 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 3). 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. The hulls are being investigated for creating higher value biobased composites using styrene-butadiene rubber and PLA as the matrix polymer.

The group is also working on engineering biobased Interpenetrating Polymer Networks (IPNs) derived from silylated soybean oil and polydimethylsiloxanes.

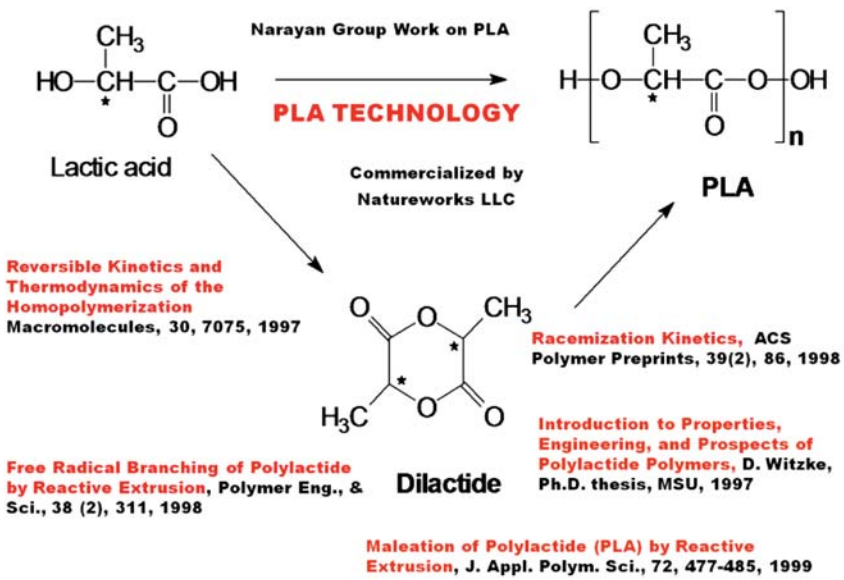



**FIGURE 2.** PLA technology commercialized by Natureworks LLC.

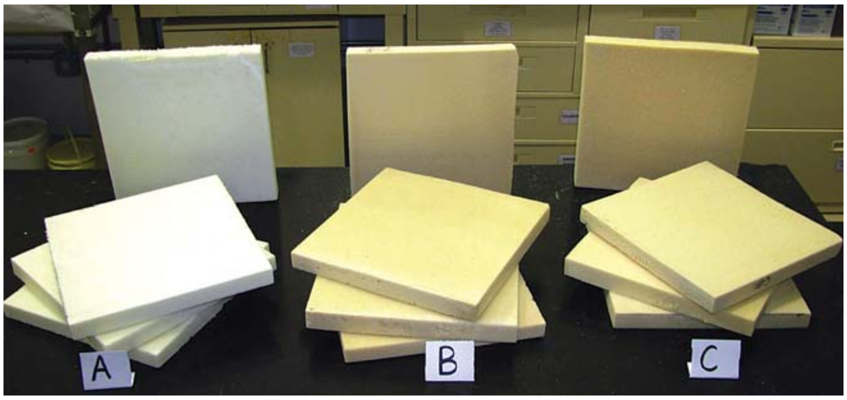



**FIGURE 3.** Samples of rigid polyurethane foams: (A) reference formulation with no soy polyol, (B) contains 25% soy polyol, (C) contains 50% soy polyol.

## RECENT PUBLICATIONS


Sudhanwa Dewasthale; Daniel Graiver; Ramani Narayan. "Biobased inter-penetrating polymers networks derived from oligomerized soybean oil and polydimethylsiloxane," *Journal of Applied Polymer Science*. 2015;132(13). (2015)

Alix Grabowski; Susan E. M. Selke; Rafael Auras; Martin K. Patel; Ramani Narayan. "Life cycle inventory data quality issues for bioplastics feedstocks," *International Journal of Life Cycle Assessment*. 2015. (2015)

Yuya Tachibana; Xiangke Shi; Daniel Graiver; Ramani Narayan. "The Use of Glycerol Carbonate in the Preparation of Highly Branched Siloxy Polymers," *Silicon*. 2014;7(1):5–13. (2014)

Elodie Hablot; Sathiskumar Dharmalingam; Douglas G. Hayes; Larry C. Wadsworth; Christopher Blazy; Ramani Narayan. "Effect of Simulated Weathering on Physicochemical Properties and Inherent Biodegradation of PLA/PHA Nonwoven Mulches," *Journal of Polymers and the Environment*. 2014;22(4):417–429. (2014)

Ramani Narayan. "The facts about biodegradable plastics," *Resource Recycling*. 2014;33(1):32–36. (2014)

Ramani Narayan. "Principles, Drivers, and Analysis of Biodegradable and Biobased Plastics," in *Handbook of Biodegradable Polymers,* 2nd Edition, Ed. Catia Bastioli; Smithers Rapra Technology, November 2014.

# Jason Nicholas

**Assistant Professor | jdn@msu.edu | 517.355.1616 | C9C Engineering Research Complex**

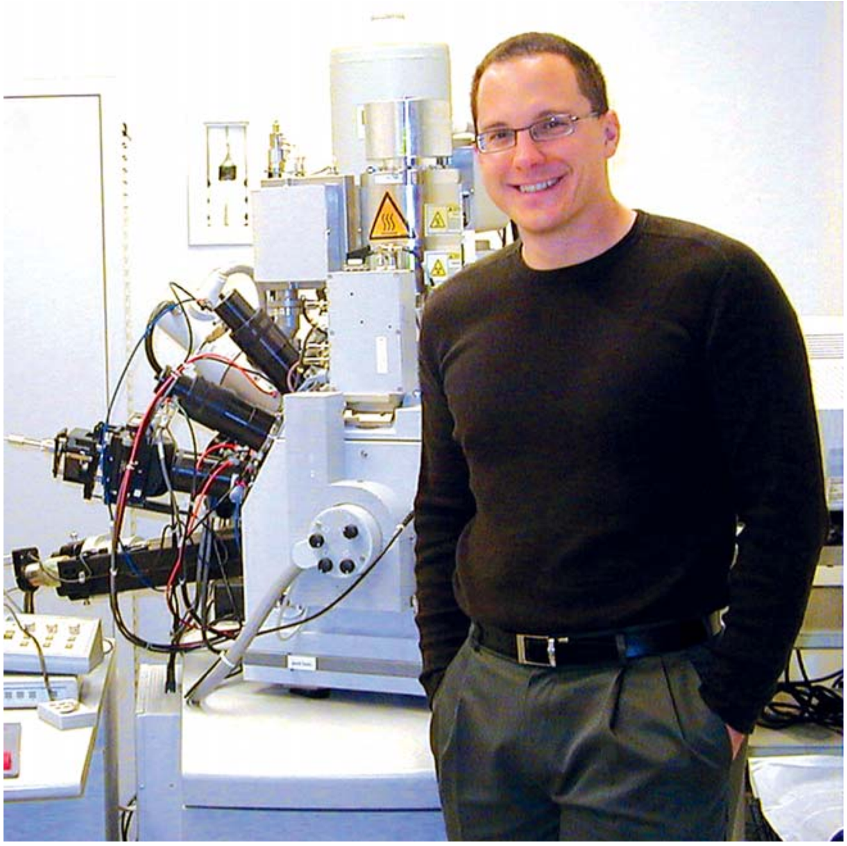


**FIGURE 1.** Prof. Nicholas in front a focused ion beam-scanning electron microscope (FIB-SEM) used to obtain 3D microstructural reconstructions.

## RESEARCH INTERESTS

Solid oxide fuel cells, mechano-chemical coupling, oxidation resistant alloys, chemical separators, chemical reactors, cost-effective processing methodologies, chemical sensors, batteries, chemical actuators, pseudo-capacitors, electro-chromic coatings, nano-composite electrode modeling, micro-structural optimization

## LAB & LOCATION

Solid State Ionics Laboratory, 172 Energy & Automotive Research Laboratory

## WEBSITE

https://www.egr.msu.edu/nicholasgroup/index.php

## SPECIAL EQUIPMENT AVAILABLE

1,200°C controlled atmosphere in situ curvature measurement system, 1,600°C controlled atmosphere dilatometer (Netzsch 402C), 1,600°C controlled atmosphere TGA-DSC (Netzsch Jupiter 449 F5)

## GROUP MEMBERS

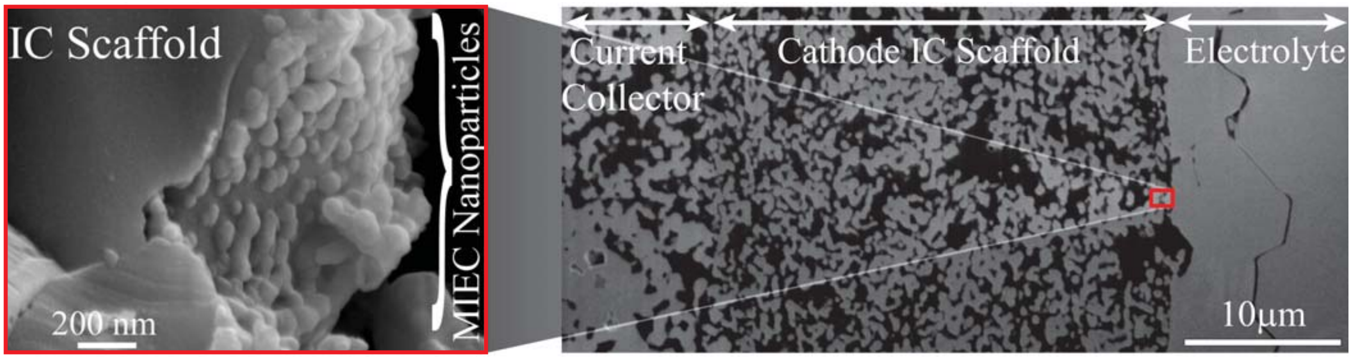
COLLABORATORS: Yue Qi, Richard Lunt, Thomas Bieler.
STUDENTS: Thedore Burye, Tridip Das, Yuxi Ma, Eric Straley, Quan Zhou, Riley O'Shea.

## CURRENT RESEARCH FOCUS

- ***Solid oxide fuel cell microstructural modelling and optimization.*** Solid oxide fuel cells (SOFCs) are a promising green energy technology offering high chemical to electricity conversion efficiencies, the ability to both store and produce energy, and a possible path to transition from today's hydrocarbon-based economy to a $CO_2$-neutral economy running on hydrogen, solar fuels, or biofuels (Nicholas 2013). Unfortunately, traditional SOFCs have been restricted to operating temperatures in excess of 750°C. To reduce realize intermediate temperature (450–700°C) SOFCs, the Nicholas Group has been seeking to understand and microstructurally tailor nano-composite solid oxide fuel cell cathodes produced via the infiltration method. In addition to discovering methods to tailor the size of the nanoparticles produced via the infiltration method (Burye and Nicholas 2015), we have developed the world's the world's most highly cited "solid oxide fuel cell infiltrated electrode performance model," the SIMPLE Model. An online SIMPLE model nano-composite cathode polarization resistance calculator with user-customizable materials combinations and electrode microstructures is available at https://www.egr.msu.edu/nicholasgroup/simple.php. Ongoing activities in this area are focused on how to control degradation and control performance under load.

- ***Curvature relaxation surface exchange measurements.*** Most electrical losses within a solid oxide fuel cell are caused by the difficulty of incorporating oxygen into the cathode material. While nano-structuring SOFC cathodes to increase surface area can result in improved performance and operating temperature reductions, in order to realize low temperature (100–400°C) operation, new materials with improved oxygen surface exchange kinetics are needed. However, before this can be realized the SOFC community needs to understand the source

**FIGURE 2.** Scanning electron micrograph of a SOFC cathode made of mixed ionic electronic conducting (MIEC) infiltrate atop an ionic conducting (IC) scaffold.



of the 1,000–10,000 times differences in the oxygen surface exchange rate coefficient reported between studies of nominally identical materials. To help advance our understanding, the Nicholas Group has developed a new curvature relaxation measurement technique that can be used to measure chemical oxygen surface exchange coefficient measurements *in situ*, under actual catalytic converter/SOFC/oxygen sensor operating conditions, without the need for stress-state/film oxygen stoichiometry altering electrodes. This technique extracts the oxygen surface coefficient from the curvature change of a film-plus-inert substrate bilayer reacting to an instantaneous change in oxygen partial pressure. This new technique has been shown to be applicable to both dense thin films and porous thick films and is the only currently available technique that simultaneously measures the oxygen surface exchange coefficient and the film stress. Ongoing activities in this area are focused on how to use film stress to control the point defect concentrations, and hence the oxygen surface exchange coefficients, of SOFC electrode materials.

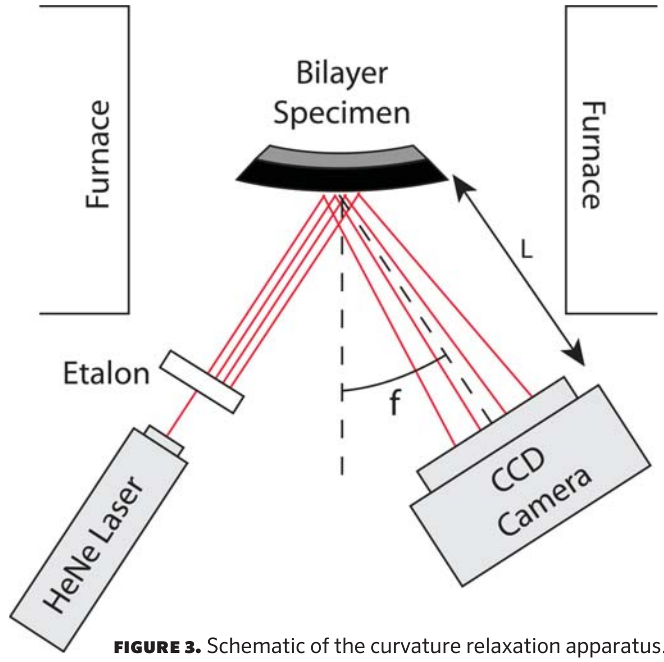


**FIGURE 3.** Schematic of the curvature relaxation apparatus.

- ***Durable, impermeable high-temperature brazes.*** Traditional Ag/CuO Solid oxide fuel cell brazes exhibit detrimental pore formation caused by wetting problems during manufacturing, the reduction of CuO, and water vapor formation within the braze. The objective of our work is to design and test new, SOFC-compatible, silver-free brazes forming durable, oxygen and hydrogen impermeable protective surface scales. Computational efforts to identify promising new braze compositions are being led by the research group of Dr. Yue Qi, while the Nicholas Group and the group of Dr. Thomas Bieler are leading experimental studies aimed at characterizing new braze and braze oxide compositions.

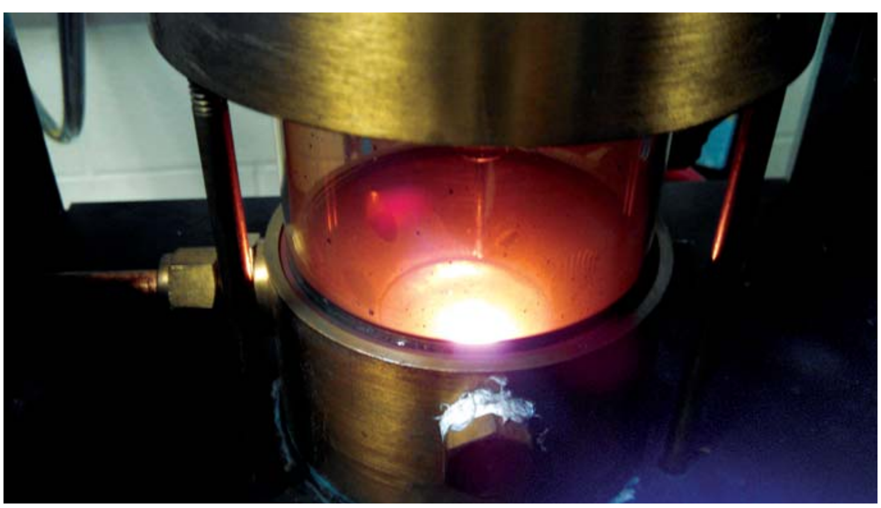


**FIGURE 4.** Arc melting of a new SOFC braze.

## RECENT PUBLICATIONS

Theodore E. Burye; Jason D. Nicholas. "Improving $La_{0.6}Sr_{0.4}Co_{0.8}Fe_{0.2}O_{3-\delta}$ infiltrated solid oxide fuel cell cathode performance through precursor solution desiccation," *Journal of Power Sources*. 2015;276:54-61. (2015)

Andrew J. Flegler; Theodore E. Burye; Qing Yang; Jason D. Nicholas. "Cubic yttria stabilized zirconia sintering additive impacts: A comparative study," *Ceramics International*. 2014;40(PB):16323–16335. (2014)

T.E. Burye; J.D. Nicholas. "Tailoring Mixed Ionic Electronic Conducting nano-particle size through desiccation and/or doped ceria oxide pre-infiltration," *ECS Transactions*. 2014;61(1):85–91. (2014)

Jason D. Nicholas; Yue Qi; Sean R. Bishop; Partha P. Mukherjee. "Introduction to mechano-electro-chemical coupling in energy related materials and devices," *Journal of the Electrochemical Society*. 2014;161(11):Y11–Y12. (2014)

Qing Yang; Jason D. Nicholas. "Porous thick film lanthanum strontium ferrite stress and oxygen surface exchange bilayer curvature relaxation measurements," *Journal of the Electrochemical Society*. 2014;161(11):F3025–F3031. (2014)

# Robert Ofoli

**Associate Professor** | **ofoli@egr.msu.edu** | **517.432.1575** | **428 S. Shaw Lane, Room 1248**

## RESEARCH INTERESTS

Sustainable chemicals/energy production: biomass to chemicals and high density liquid fuels; biomimetic hydrogen generation

## LAB LOCATION

2256 Engineering Building

## WEBSITE

http://www.egr.msu.edu/people/profile/ofoli

## SPECIAL EQUIPMENT AVAILABLE

CHI 660D electrochemical workstation

## GROUP MEMBERS

STUDENT: Hao Yuan. COLLABORATING FACULTY: Gary Blanchard (Chemistry), Don Cropek (U.S. Army CERL, Urbana-Champaign), Alvin Holder (Chemistry, Old Dominion), James Jackson (Chemistry), Richard Lunt, Dennis Miller, Yirong Mo (Chemistry, Western Michigan), Sherine Obare (Chemistry, Western Michigan), Yue Qi.

## PATENTS GRANTED

Worden, R.M.; Ofoli, R.Y.; Hassler, B.L.; Kohli, N.; Lee, I. Customizable and Renewable Nanostructured Interface for Bioelectronics Applications. US Patent 8,435,773, May 7, 2013.

## CURRENT RESEARCH FOCUS

Our research addresses the use of nanoscale catalysts and biomimetic catalysts to produce chemicals and high-density liquid fuels. Our goal is to integrate rational catalyst design and synthesis, characterization and assessment, and modeling and simulation to understand the structure-function relationships. We currently focus on two areas of significant scientific and societal interest: biomimetic water oxidation to produce hydrogen and organic materials; and catalytic transformation of biorenewables to chemicals and high-density liquid fuels equivalent to those from petroleum-based sources.

- ***Biomimetic water oxidation to produce hydrogen fuel.*** Solar energy can meet the global demand for energy. However, it has the significant drawback that it is intermittent. Fortunately, this can be mitigated by effective strategies for its storage. Artificial photosynthesis (AP), a mimic of the natural photosynthesis process, provides a promising mechanism for solar energy storage through the splitting of water into oxygen and hydrogen ions. The hydrogen ions can be subsequently reconstituted to obtain hydrogen gas. An even more practical route is to combine water oxidation with carbon dioxide sequestration to produce organic chemicals and liquid fuels. An important objective of our work is to develop photoanode complexes that integrate manganese-based catalysts with low-cost solar energy collection to induce water oxidation without external energy input. This collaborative project has four integrated components: synthesis, characterization and assessment of a biomimetic manganese-based water oxidation catalysts; development of an integrated device for solar energy collection and direct conversion to electrical energy to power the process; *ab initio* work to provide structural, thermodynamic and kinetic insights to guide both catalyst synthesis and photoanode development; and proof of concept demonstration to produce organic fuels.

  This work aims to develop catalytic systems that enable reuse. We have successfully anchored catalysts to various conductive surfaces to enable recycling, while ensuring that the catalyst remains active. We have compared the functionality of a mimic of the oxygen evolution complex (OEC) $[Co4(\mu_3\text{–}O)_4(\mu\text{–}O_2CMe)_4(py)_4]$ in solution to that of the same catalyst anchored to a conductive surface. The experimental results provide clear evidence that the catalyst can be successfully immobilized on ITO by electrochemical deposition, and that it functions in the same manner as it does in solution. This study also demonstrated that the current density profile for deposition of a catalyst synthesized *ex situ* is similar to that of heterogeneous catalysts produced by *in situ* synthesis. However, the separation

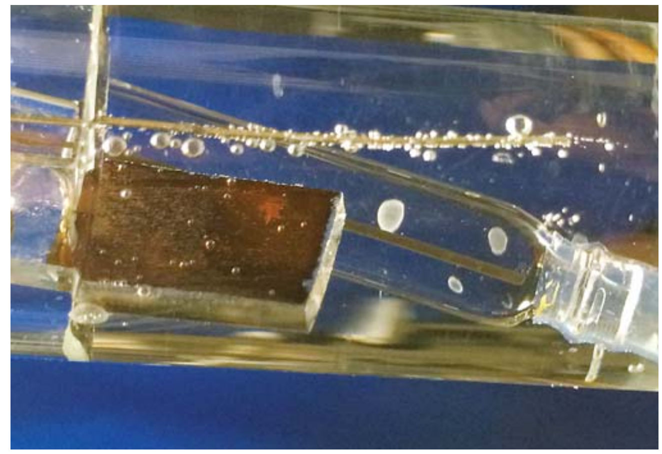


**FIGURE 1.** Evidence of $O_2$ bubbles from an anode wire during water oxidation experiment using MnOx.

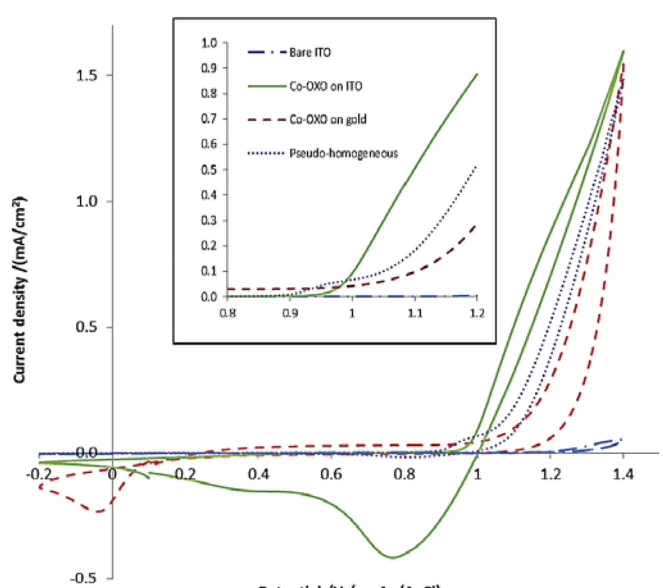



**FIGURE 2.** Cyclic voltammograms acquired at a scan rate of 0.01V/s on bare ITO (blue dash dot), Co-OXO immobilized on gold (red dashed line) and Co-OXO immobilized on ITO (green solid line) in PBS buffer at pH = 7.0.

of catalyst synthesis and immobilization into separate functions has the potential to enable a more systematic optimization of the resulting complex.

COLLABORATORS: Richard Lunt, Yue Qi. EXTERNAL: Don Cropek, Alvin Holder

- ***Catalytic transformation of biorenewable materials to produce high-density liquid fuels.*** Global energy needs are expected to increase significantly in the near future. Even with new sources made possible by such technologies as fracking, it is generally believed that future petroleum supplies will not meet global needs. This has created a critical need for the sustainable production of fuels and chemicals. tSolar energy is an important source for meeting global demand, because of the qunatity incident on the planet. However, even if technological challenges are addressed to make solar energy a mainstream source, it will likely not meet the demand for high-energy-density liquid fuels. This will, instead, fall on biomass conversion and subsequent exhaustive reduction. The transformations required are well-developed for petroleum processing, but core chemical differences between crude oil and biomass prevent direct application to bioprocessing. To help address this significant global issue, our group of collaborators is working on four coordinated activities: (1) synthesis, *in situ* characterization, and assessment of bimetallic nanocatalyst complexes that promote optimum reactivity; (2) focus on the three most important elementary bio-transformations: deoxygenation, decarboxylation, and hydrogenation; (3) assessment of catalytic complexes in executing pre-selected sequences of elementary reactions to convert selected biomaterials to target intermediate or final products; and (4) *ab initio* computational work to help understand catalytic behavior in model bimetallic structures.

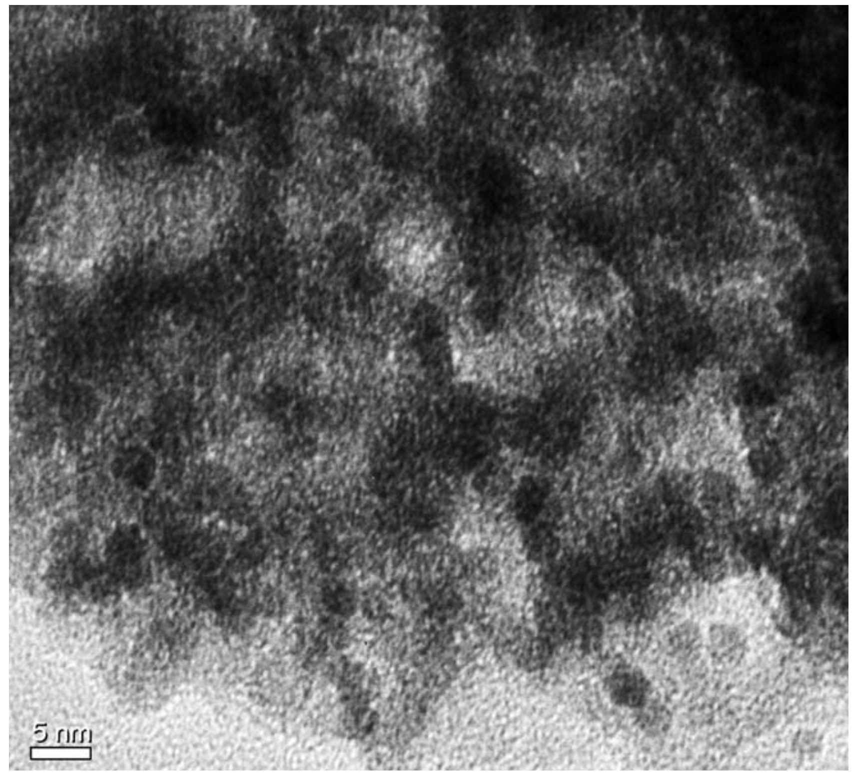



**FIGURE 3.** HRTEM images of RuNPs on MSU-F at a magnification of 300K (scale bar = 5 nm).

We expect the successful completion of this project to provide a transformational and transferable platform for generating value-added chemicals and high energy-density liquid fuels equivalent to those from crude oil.

COLLABORATORS: Gary Blanchard, James Jackson, Dennis Miller, Yirong Mo, Sherine Obare

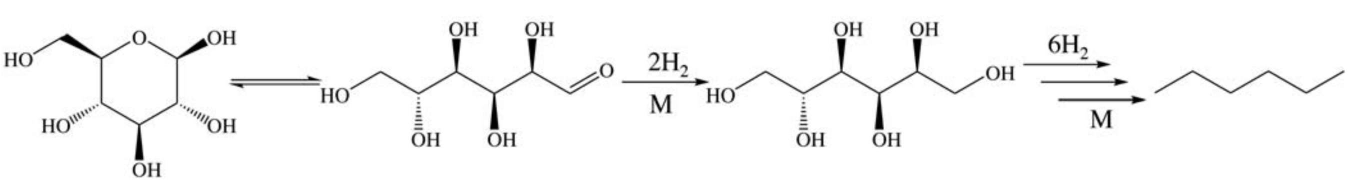


**FIGURE 4.** Schematic reaction pathway for exhaustive reduction of a saccharide to hexane.

## RECENT PUBLICATIONS

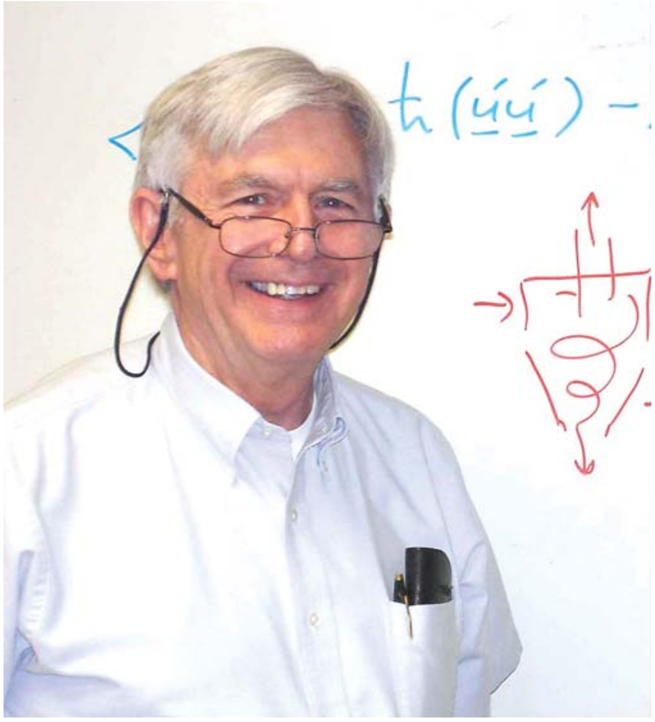
Hao Yuan; De'Andra L. Newton; Luke A. Seymour; Anja Metz; Donald Cropek; Alvin A. Holder; Robert Y. Ofoli. "Characterization and functional assessment of a cobalt(III)-oxo cubane cluster water oxidation catalyst immobilized on ITO," *Catalysis Communications*. 2014;56:76–80. (2014)

Xianfeng Ma; Rui Lin; Christopher Beuerle; James E. Jackson; Sherine O. Obare; Robert Y. Ofoli. "Effects of surface activation on the structural and catalytic properties of ruthenium nanoparticles supported on mesoporous silica," *Nanotechnology*. 2014;25(4). (2014)

Jared T. Wabeke; Clara P. Adams; Setare Tahmasebi Nick; Liyana A. Wajira Ariyadasa; Ali Bolandi; Darryl W. Corley; Robert Y. Ofoli; Sherine O. Obare. "Biofuels and high value added chemicals from biomass using sustainably prepared metallic and bimetallic nanoparticles," *RSC Green Chemistry*. 2013:157–189. (2013)

# Charles Petty

**Professor | petty@msu.edu | 517.353.5486 | 428 S. Shaw Lane, Room 1245**



### 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

### COLLABORATING STUDENTS

Andrew Bowden (Chemical Engineering, Undergraduate Professorial Assistant),Devinda Wijewardena (Chemical Engineering, Undergraduate Professorial Assistant), Abdul Motin (PhD Candidate, Mechanical Engineering).

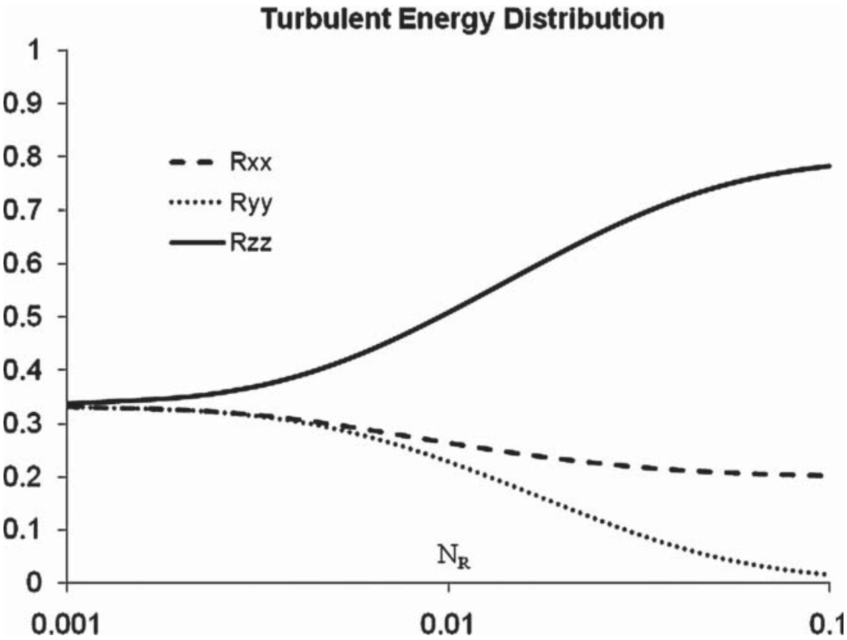



**FIGURE 1.** Redistribution of turbulent kinetic energy among the three components of the velocity in rotating shear flows. (Karuna S. Koppula, PhD Dissertation, MSU, 2009).

### COLLABORATING FACULTY & COLLEAGUES

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

### PATENTS GRANTED

Petty, C.A.; Dvorak, R.G.; Chen, H.C. (Michigan State University). Improved Hydrocyclone. US Patent 4855066, 1989.

### RESEARCH INTERESTS

- ***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 twenty 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 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 in 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.

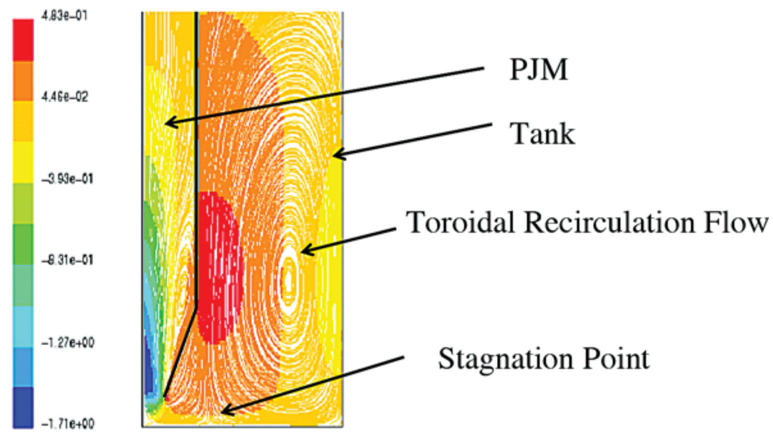



**FIGURE 2.** Path lines colored by axial velocity (m/s) at 5 seconds into Cycle 4 (suction phase). Note the toroidal secondary flows within the PJM as wall as in the tank. (Dina A. Eldin, Master of Science Thesis, MSU, 2003).

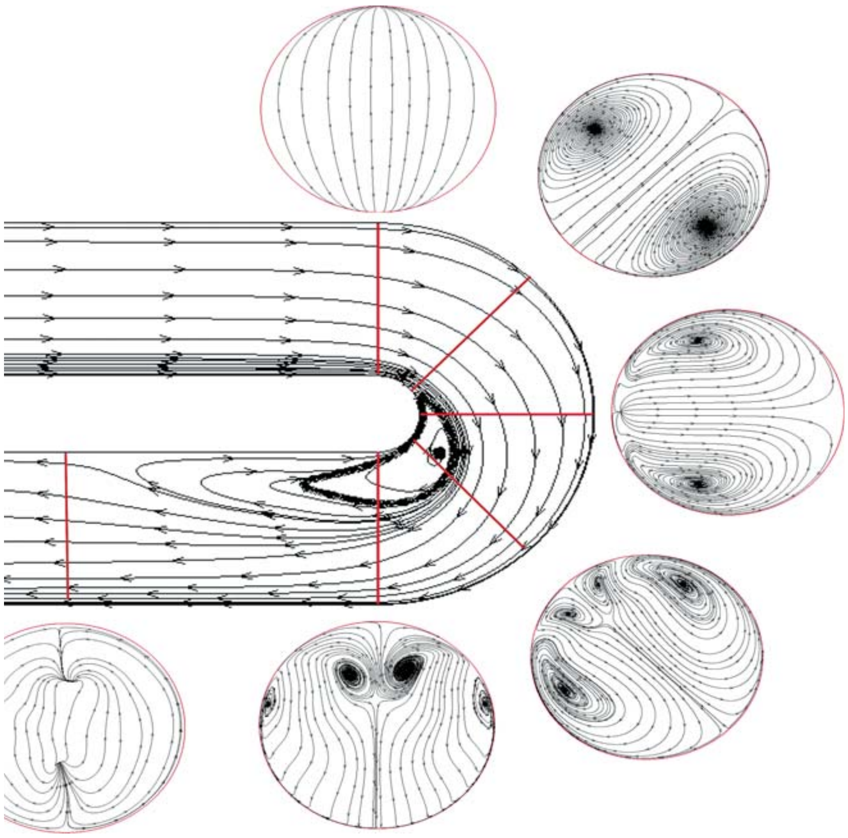


**FIGURE 3.** Flow patterns through a bend (180°) with cutouts that show various recirculation patterns at different cross-sections. The turbulence model and the wall functions strongly influence the qualitative accuracy of the simulation. (Pusheng Zhang,PhD Dissertation, MSU, 2013).

## RECENT PUBLICATIONS

YoChan Kim; Andre Benard; Charles A. Petty, “Microstructure and Rheology of Rigid Rod Suspensions,” *Ind. Eng. Chem. Res.*, DOI:10.1021/ie503995y, 20 Jan. 2015.

Abdul Motin; Volodymyr V. Tarabara; Charles A. Petty; André Bénard. “Computational study of the effects of the conical chamber design on the internal flow structures within a hydrocyclone,” 2014 Conference Proceedings: Oil and Gas and Chemical Filtration and Separations, AFS 2014. 2014:542–553. (2014)

Karuna S. Koppula; Satish Muthu; André Bénard; Charles A. Petty. “The URAPS closure for the normalized Reynolds stress,” *Physica Scripta*. 2013;88(T155). (2013)

# Yue Qi

**Associate Professor | yueqi@egr.msu.edu | 517.432.1243 | 428 S. Shaw Lane, Room 3509**

**RESEARCH INTERESTS**
Computational Materials Science

**LAB & LOCATION**
Materials Simulation for Clean Energy (MSCE) Lab, 428 S. Shaw Lane, Room 1260

**WEBSITE**
http://researchgroups.msu.edu/msce

**SPECIAL EQUIPMENT AVAILABLE**
Dedicated computer clusters at the MSU High Performance Computing Center

**GROUP MEMBERS**
Tridip Das, Christine James, Kwang Jin Kim, Yuxiao Lin, Jialin Liu, Dr. Sung Yup Kim

**PATENTS GRANTED**
Qi, Y. Machining of aluminum surfaces. US Patent 8057133, November 15, 2011.
Qi, Y.; Yuen, P. Coated seal for sealing parts in a vehicle engine. US Patent 7968167, June 28, 2011.

**CURRENT RESEARCH FOCUS**
***Computational design of materials atom-by-atom accelerates materials discovery for batteries and fuel cells via multi-scale simulations.***

At the Materials Simulation for Clean Energy (MSCE) Lab, Qi and her group develop multi-scale simulation methods to design materials *atom by atom*. We are interested in materials that deliver clean energy, such as Li-ion batteries, fuel cells, and lightweight materials. Utilizing the High Performance Computer Center (HPCC) at MSU and both commercial and homemade software, we are specialized at designing materials from their atomic structures. We screen materials chemistry with first-principles methods, which solve the fundamental quantum mechanical equations of matter to calculate accurately the properties that are difficult to measure experimentally. We simulate materials behavior that involves millions of atoms using molecular dynamics with faster and accurate atomic interactions (force field). We have successfully integrated nano-scale insights learned from atomic simulations into meso- and micro-structures, governed by continuum theories, to design materials that are important for energy-efficient and sustainable transportation industry. Central to these applications is a combination of "top-down" and "bottom-up" multi-scale modeling strategies with an associated experimental/modeling research program. Therefore, most of our projects have strong collaboration with experimental groups and industry.

Currently, on-going projects include:

- ***Electron and ion transport in complex materials and interphases.*** Defect-mediated diffusion greatly affects the power performance of battery and fuel cell devices. Using density functional theory (DFT) informed thermodynamics, we can identify the dominant diffusion carriers and their diffusion pathways as a function of voltage, pressure, temperature, and strain. Thus, new materials with dopants can be tested and operating conditions can be optimized. Currently, we are designing high-energy-density cathode materials and artificial solid electrolytes interphase (SEI) preventing capacity loss for Li-ion batteries. We also design catalyst at desired strain for low-temperature solid oxide fuel cells.

- ***Predicting chemical-mechanical degradation in Li-ion batteries.*** In order to computationally screen and design future

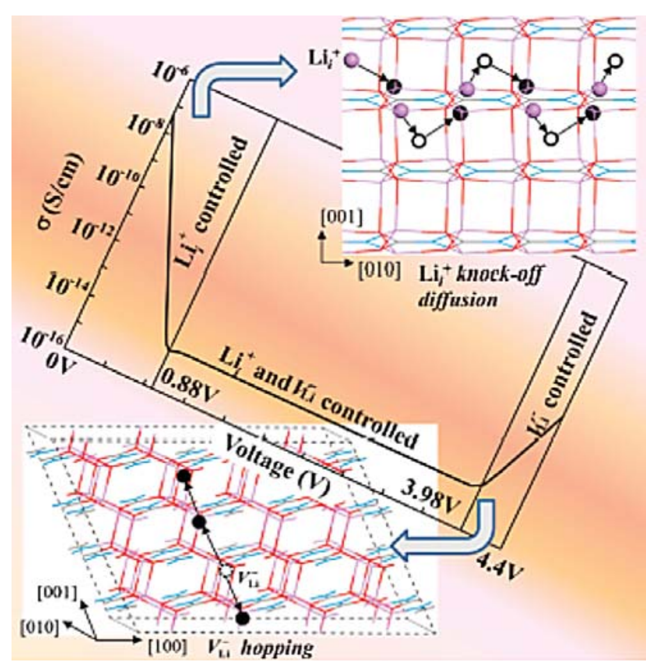



**FIGURE 1.** Direct calculation of diffusion carriers and ionic conductivity in $Li_2CO_3$ as a function of voltage.

battery materials for improved durability, we need to be able to predict failure starting from materials' properties and structures without using non-physical fitting parameters.

We have used DFT to predict elastic and fracture properties of electrode materials and their interfaces integrated into meso-structures to predict the lithiation-induced stress and failure of composite electrodes. Many of our predictions have been confirmed by *in situ* experiments. Currently, we are integrating structural evolution and chemical degradations into a battery predictive life model. We are using these methods to develop high-capacity and long-lasting nano-structured electrodes.

- ***The impact of environment on forming and machining lightweight materials.*** The environment (air, water, solution, electrolyte) can have a profound impact on deformation processes for lightweight metals (Al, Mg, Ta, Li, etc.) that have a high affinity to oxygen. Similar impacts of the environment are seen for electrode materials. One can further imagine that as the characteristic size of these materials shrinks, surface reactions will contribute more and more, likely changing substantially the mechanical properties of the nano-device. By developing a reactive molecular dynamics method, we demonstrated how oxidation changes the deformation and failure mechanism in a nano-scale device, for example in an Al nano-wire. The nano-scale mechanisms also have a profound impact in large scale manufacturing processing, such as the tribology and surface quality of Al sheets for car panels made with hot forming processes.

- ***We are further addressing environmental effects for a variety of problems.*** Examples include: How Mg fractures differently in air and vacuum; why nano-crystalline $Al_2O_3$ appears to be superplastic when oxygen diffuses into the grain boundaries; under what conditions do diamond-like carbon films become almost frictionless in a $H_2$ or $H_2O$ environment; and how to ensure an always-passivated surface.

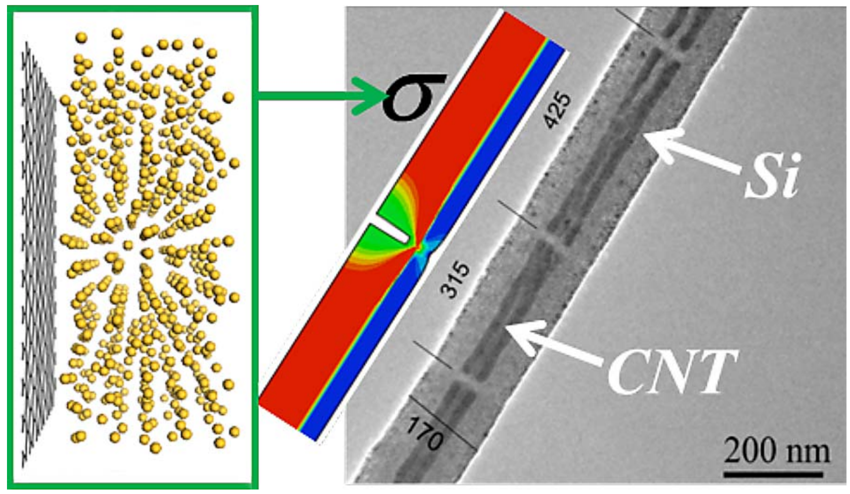



**FIGURE 2.** Design of always-conducting Si-CNT nanostructure. The weak Si/CNT interface contributes to cracks in Si (as seen in the computed stress field model and by situ-TEM).

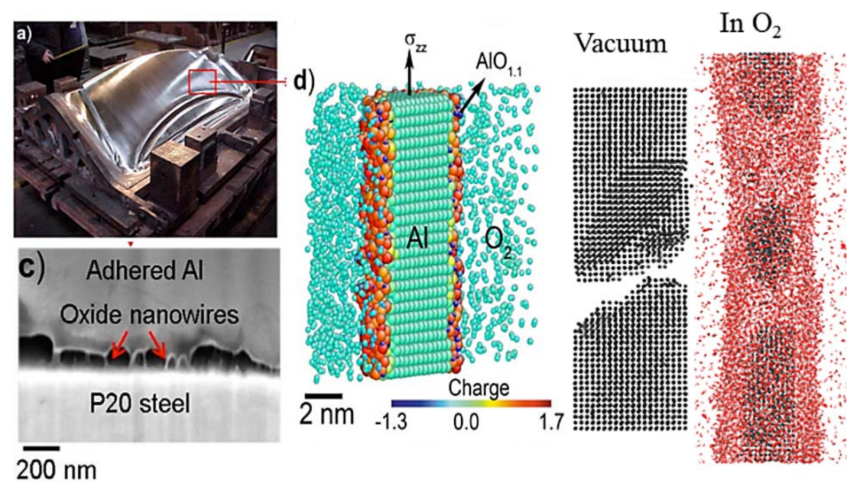



**FIGURE 3.** During hot-forming of Al-Mg alloy to make the lift gate of a car, nanowires were formed at adhered interfaces. Reactive molecular dynamics shows that Al nanowire deformation is drastically different in vacuum and $O_2$.

## RECENT PUBLICATIONS


Sheng Sun; Yue Qi; Tong-Yi Zhang. "Dissecting graphene capacitance in electrochemical cell," *Electrochimica Acta*. 2015;163:296–302. (2015)

Shutian Yan; Xinran Xiao; Xiaosong Huang; Xiaodong Li; Yue Qi "Unveiling the environment-dependent mechanical properties of porous polypropylene separators," (United Kingdom). 2014;55(24):6282–6292. (2014)

Fatih G. Sen; Ahmet T. Alpas; Adri C. T. Van Duin; Yue Qi. "Oxidation-assisted ductility of aluminium nanowires," *Nature Communications*. 2014;5. (2014)

Maria E. Stournara; Yue Qi; Vivek B. Shenoy. "From Ab initio calculations to multiscale design of Si/C core-shell particles for Li-ion anodes," *Nano Letters*. 2014;14(4):2140–2149. (2014)

D.J. Oliver; W. Paul; M. El Ouali; T. Hagedorn; Y. Miyahara; Y. Qi; P.H. Grütter. "One-to-one spatially matched experiment and atomistic simulations of nanometre-scale indentation," *Nanotechnology*. 2014;25(2). (2014)

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Jianchao Chen; Yongda Yan; Tao Sun; Yue Qi; Xiaodong Li. "Probing the roles of polymeric separators in lithium-ion battery capacity fade at elevated temperatures," *Journal of the Electrochemical Society*. 2014;161(9):A1241–A1246. (2014)

Yue Qi; Louis G. Hector; Christine James; Kwang Jin Kim. "Lithium concentration dependent elastic properties of battery electrode materials from first principles calculations," *Journal of the Electrochemical Society*. 2014;161(11):F3010–F3018. (2014)

Sung-Yup Kim; Yue Qi. "Property evolution of Al2O3 coated and uncoated Si electrodes: A first principles investigation," *Journal of the Electrochemical Society*. 2014;161(11):F3137–F3143. (2014)

# S. Patrick Walton

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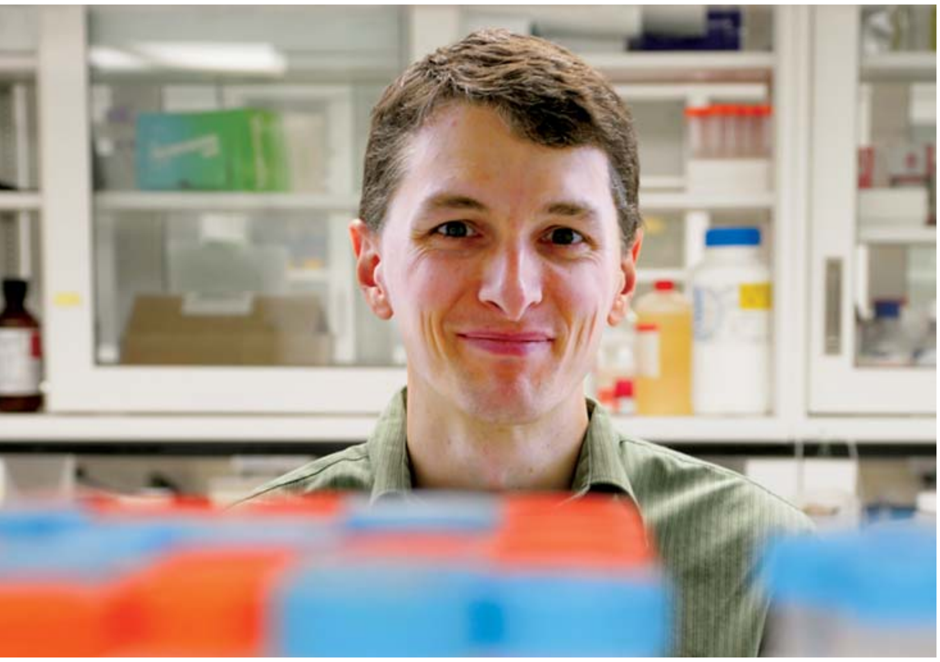

### RESEARCH INTERESTS

Biomolecular engineering and biotechnology

### LAB & LOCATION

Applied Biomolecular Engineering Laboratory, 428 S. Shaw Lane, Room 2125

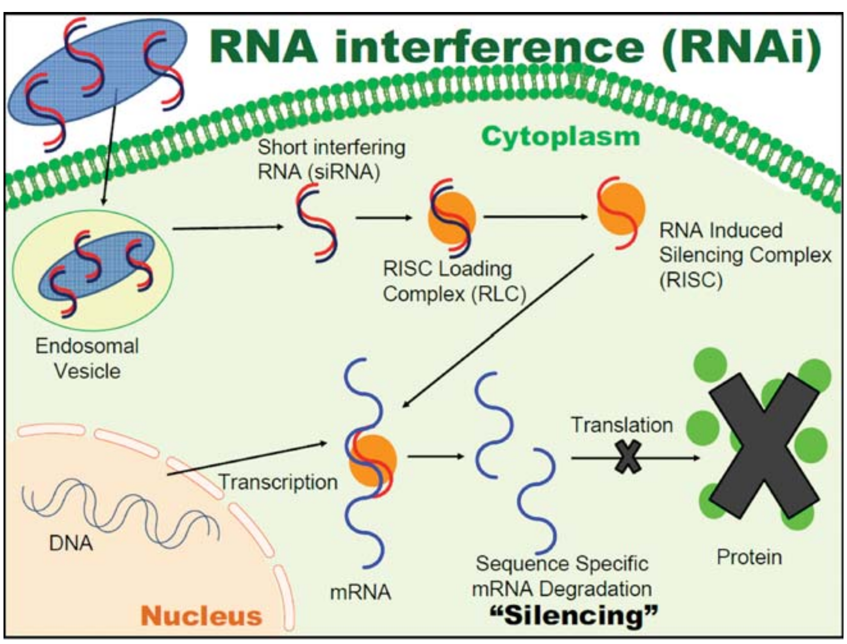


**FIGURE 1.** *RNA interference.* RNA interference is initiated upon successful delivery of an siRNA into cells. Upon release from the delivery vehicle and entry to the cytoplasm, siRNAs are bound by a complex of proteins, Dicer, TRBP, and Ago2, known collectively as the RISC loading complex (RLC). The active RNA Induced Silencing Complex (RISC) then utilizes one strand of the siRNA, the guide strand, to bind the target mRNA by complementarity, leading to sequence specific degradation of the mRNA and a subsequent reduction in protein expression.

### WEBSITE

http://www.egr.msu.edu/abel/

### SPECIAL EQUIPMENT AVAILABLE

Fluorescent and chemiluminescent imaging, cell culture facilities

### GROUP MEMBERS

GRADUATE STUDENTS: Phil Angart, Daniel Vocelle; UNDERGRADUATE STUDENTS: Rebecca Carlson, Kwasi Adu-Berchie, Alex van Fossen, Rebecca Gorz

### CURRENT RESEARCH FOCUS

One achievable goal of the 21st century is "personalized medicine," the design of diagnostics and therapeutics specifically for a single patient. Reaching this goal depends on the development of new diagnostic approaches that can acquire vast quantities of data simultaneously, improving our understanding of the behavior of diseased cells, and therapeutics that can be delivered specifically to the diseased cells and can target the molecular-scale causes of the disease with exceptional activity and specificity.

The Applied Biomolecular Engineering Laboratory (ABEL), led by S. Patrick Walton, is currently working in both these areas, specifically on technologies that rely on nucleic acids (i.e., DNA and RNA). Areas of investigation include: (1) designing nucleic acid-based therapeutics based on understanding their mechanism of action, and (2) developing diagnostics to measure protein levels in parallel, improving the understanding of cellular responses to stimuli. Recent work involves investigating how proteins interact with a new class of therapeutics, short, interfering RNAs, moving towards guidelines for designing these molecules. Additionally, the ABEL is developing a technique for parallel measurements of transcription factors, proteins that help the cell respond to stimuli, using a solution-phase magnetic bead-based approach.

The ABEL is focused on the analysis and application of nucleic acid-based technologies. Our goals are the understanding of critical biophysical and biochemical parameters involved in these processes and, in turn, the tuning of these parameters to achieve an improved

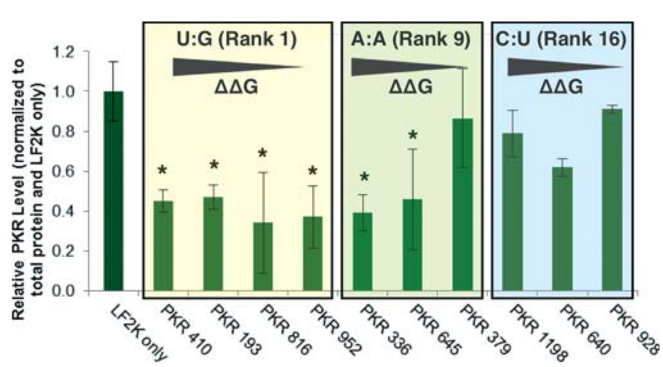


**FIGURE 2.** *Silencing of PKR by selected siRNAs.* HepG2 cells were reverse-transfected with 100 nM of siRNA for 48 h using Lipofectamine 2000 (LF2K). Results are normalized to both total protein level and PKR level of LF2K-only treated control cells (black). siRNAs were grouped by terminal nucleotide classification rank, U:G (yellow), A:A (green), and C:U (blue). Error bars = ±1 standard deviation, $n = 3$. Stars indicate a significant difference ($p < 0.05$) when compared to LF2K only treatment.

technology. The current focus of the lab is a mechanistic analysis of RNA interference (RNAi) and siRNA delivery.

Our goal in studying RNAi is to understand the factors that influence the activity of the active molecules in the pathway, short, interfering RNAs (siRNAs). We have shown that two factors, terminal nucleotide classification and terminal hybridization stability (ΔΔG), are predictive of active siRNAs (Figure 2). We are currently studying the interactions of siRNAs with RNAi pathway proteins to determine how these factors result in differential siRNA activities. Principally, we are examining the difference in activity between the two strands of an siRNA, their functional asymmetry. These studies contribute to our goal of designing siRNAs with perfect functional asymmetry, i.e., 100% activity of only the intended guide strand.

Unfortunately, designing a highly-active siRNA does not alone guarantee its function. Prior to initiating silencing, siRNAs must first enter the targeted cells by a mechanism that allows them to be active. The uptake pathways that result in maximal siRNA function are poorly understood. We are currently investigating the properties of siRNA delivery vehicles, in particular silica nanoparticles (NPs), that result in highly efficient delivery and subsequent silencing (Figure 3).

To date, we have primarily used microscopy for analyzing siRNA uptake following transfection (Figure 4). It is clear from these experiments that many delivery vehicles transport siRNAs to cells but that reaching the cells alone is insufficient to achieve silencing. Also, we have seen what appears to be recycling of degraded material out of the cells (Figure 4), further reinforcing that uptake alone may be insufficient for siRNA activity. Thus, studies on the uptake pathways for siRNAs by cells are essential for design of vehicles to transport siRNAs into cells.

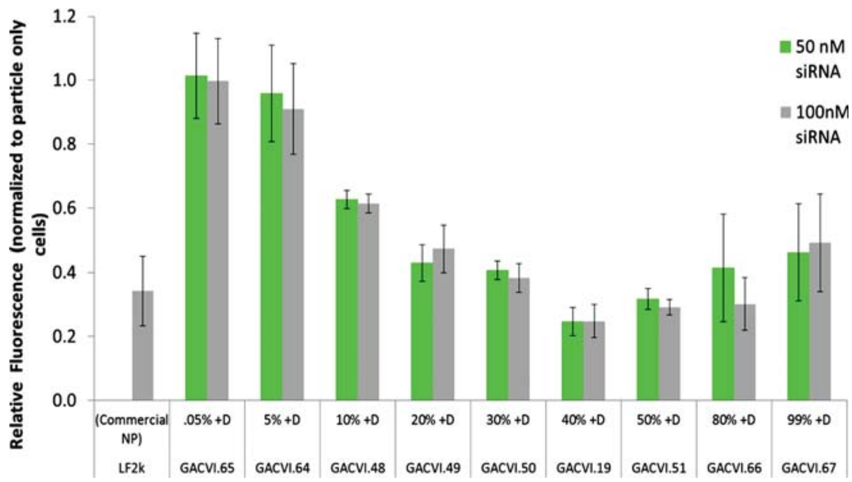


**FIGURE 3.** *Effect of NP amine content on siRNA activity.* While delivery with silica NPs results in silencing by siRNAs (% values indicate increasing amine added to the NP synthesis), none of the NPs effectively delivered plasmid (data not shown). This strongly suggests that different design rules must be applied for siRNA and plasmid delivery vehicles.

Financial support was provided in part by Michigan State University, the National Science Foundation (CBET 0941055), the National Institutes of Health (GM079688, RR024439, GM089866), the Michigan Universities Commercialization Initiative (MUCI), and the Center for Systems Biology.

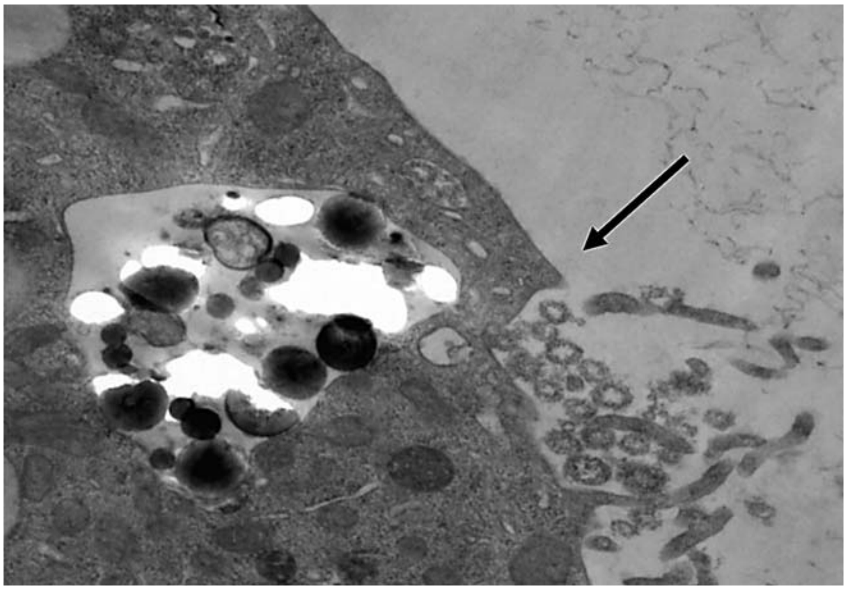

**FIGURE 4.** *TEM of cells transfected with siRNAs using solid NPs.* Silica NPs are taken up by cells and accumulate in vesicles where they appear to degrade. Particle "shells" appear to be recycled out of the cells (*arrow*). It is unclear if degradation occurs before, during, or after siRNA release.

## RECENT PUBLICATIONS


Daniel A. Lynam; Dena Shahriari; Kayla J. Wolf; Phillip A. Angart; Jacob Koffler; Mark H. Tuszynski; Christina Chan; Patrick Walton; Jeffrey Sakamoto. "Brain derived neurotrophic factor release from layer-by-layer coated agarose nerve guidance scaffolds," *Acta Biomaterialia.* 2014. (2104)

Amanda P. Malefyt; Ming Wu; Daniel B. Vocelle; Sean J. Kappes; Stephen D. Lindeman; Christina Chan; S. Patrick Walton. "Improved asymmetry prediction for short interfering RNAs," *FEBS Journal.* 2014;281(1):320–330. (2104)

Timothy J. Hinds; Patrick Walton; Mark Urban-Lurain; Daina Briedis. "Influence of integrated academic and co-curricular activities on first-year student success," ASEE Annual Conference and Exposition, Conference Proceedings. 2014. (2104)

# Tim Whitehead

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**RESEARCH INTERESTS**

Biomolecular design and engineering/renewable bioproducts/protein therapeutics

**LAB LOCATION**

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**WEBSITE**

http://www.egr.msu.edu/whitehead-lab/

**GROUP MEMBERS**

POSTDOC: James Stapleton. GRADUATE STUDENTS: Matthew Faber, Carolyn Haarmeyer, Justin Klesmith, Caitlin Kowalsky, Emily Wrenbeck.

**PATENTS GRANTED**

Baker, D.; Fleishman, S.J.; Whitehead, T.A. Polypeptides for treating and/or limiting influenza infection. US Patent 8765686, July 1, 2014.

Whitehead, T.A.; Clark, D.S.; Robb, F.T.; Laksanalamai, P.; Jiemjit, A. Heterologous expression of extremophile heat shock proteins and chaperones in microorganisms to increase tolerance to toxic compounds. US Patent 8685729, April 1, 2014.

**CURRENT RESEARCH FOCUS**

***Biomolecular design and engineering.***

Engineering life is a broad-stated goal of the new generation of biological engineers. To better accomplish this goal, these engineers pursue the ability to design novel functions rather than rely on a catalog of 'parts' culled from nature. Proteins, one of the main categories of parts, are wondrously complex biomolecules comprised of thousands of atoms, which fold into tertiary structures necessary for function by balancing competing inter- and intra-molecular

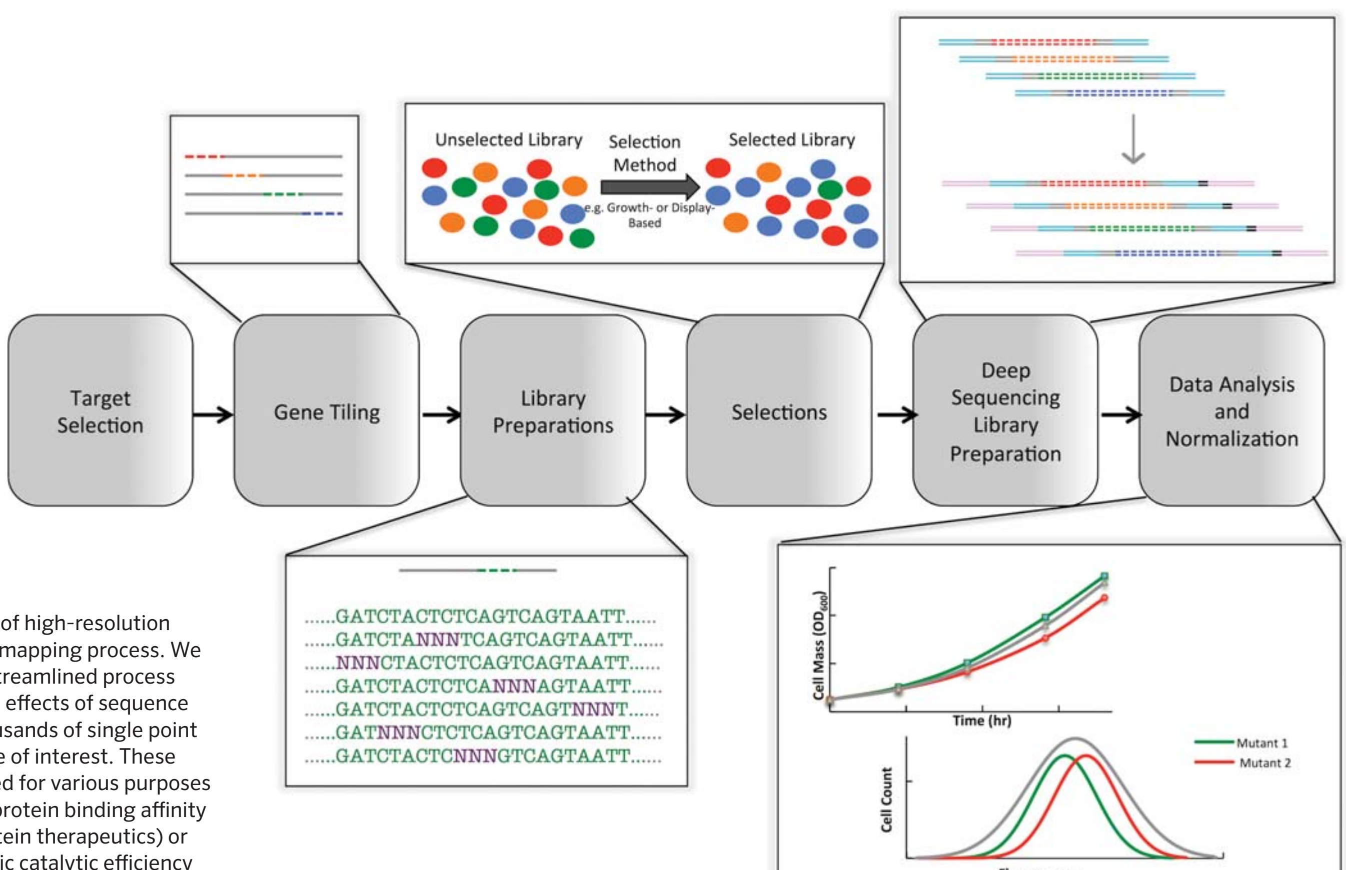


**FIGURE 1.** Overview of high-resolution sequence-function mapping process. We have developed a streamlined process for determining the effects of sequence on function for thousands of single point mutants in the gene of interest. These portraits can be used for various purposes such as improving protein binding affinity and specificity (protein therapeutics) or improving enzymatic catalytic efficiency (biomass deconstruction to biofuels).

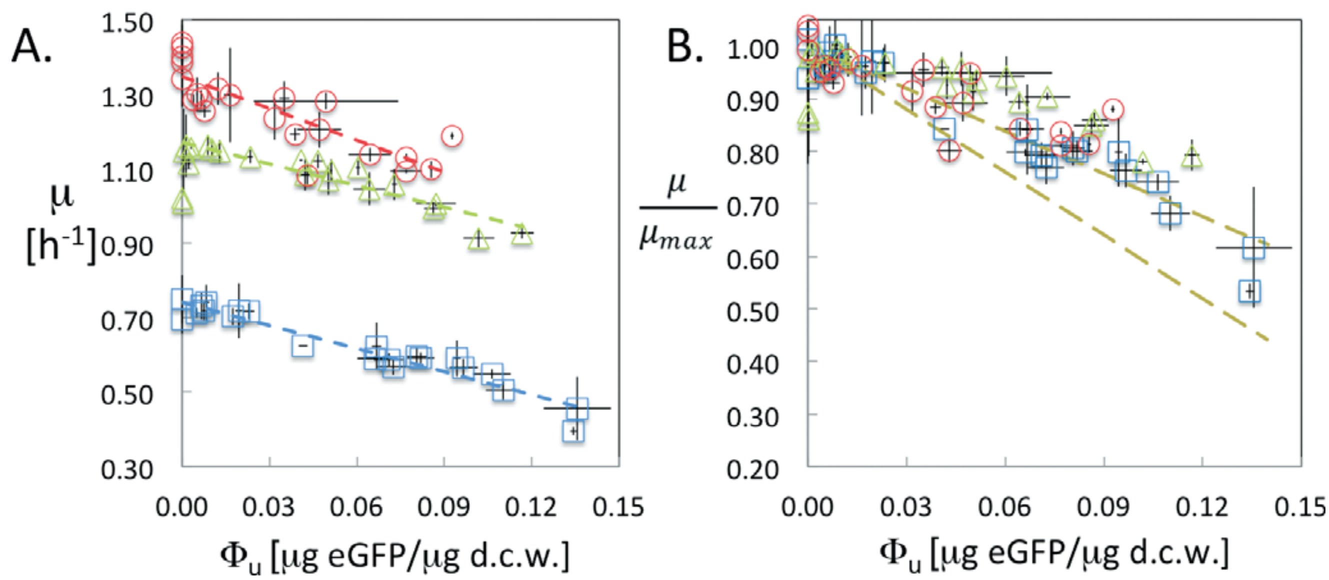


**FIGURE 2.** Amount of protein expression determines bacterial growth rates. We have validated a scaling law relating protein expression amount to growth rate. Panel A shows growth rate (*m*) as a function of eGFP mass fraction of dry cell weight (d.c.w) for different growth conditions. Panel B shows the results of Panel A normalized by maximum growth rate (mmax). The dashed lines indicate prediction from the scaling law.

forces. Imparting novel and specific functions into proteins is a difficult problem because protein structures are only marginally stable, protein structure-function relationships are not well understood, and many targeted small molecule substrates differ by as little as a single hydroxyl group or a methyl bond. The net result is that efforts to engineer or design new/improved proteins are either empirical in nature or suffer from low success rates, frustrating efforts to rationally and reliably redesign components for cellular life.

My group works to solve the problem of engineering proteins. We use and develop computational techniques to design proteins for new functions, have pioneered experimental approaches to comprehensively assess the effect of a protein's sequence on its desired function, and have imparted evolutionary and computational ideas to formulate efficient routes to optimize protein function. We also pose and experimentally validate scaling laws in biology. We are now interested in developing proteins for diverse applications like *vaccine design* and *creating the next generation of biofuels.* Our laboratory is funded by several State and Federal agencies, including the National Institutes of Health, the National Science Foundation, and the Department of Energy.

Recent highlights from the lab include:

- ***High-resolution sequence-function mapping of full proteins.*** The amino acid sequence of a protein defines its function, yet our understanding of the contribution of each amino acid to overall activity remains incomplete. As a result, current computational and experimental methods of designing functional proteins have success rates significantly less than 10%. Comprehensive sequence-function mapping involves detailing the fitness contribution of every possible single mutation to a gene by comparing the abundance of each library variant before and after selection for the phenotype of interest (Figure 1). We have extended the scope of sequence-function maps to entire protein sequences with a modular, universal sequence tiling method. We demonstrate the approach with both growth-based selections and FACS screening, offer parameters and best practices that simplify design of experiments, and present analytical solutions to normalize data across independent selections. Using this protocol, sequence-function maps covering full sequences can be obtained in four to six weeks.

- ***A simple scaling law governs bacterial growth rate as a function of protein expression.*** In exponentially growing bacteria, expression of heterologous protein impedes cellular growth rates. Recently, a scaling law was proposed that could be used to quantitatively predict this dependence. This model had no free parameters and suggested a surprising simplicity of bacterial growth rates. We tested this scaling law using synthetic promoters to drive expression of two different heterologous proteins in *E. coli* under different growth conditions. In all cases, the growth rate dependence on protein expression was consistent with this scaling law (Figure 2). Because these results validate the quantitative prediction of the fitness cost upon protein expression, we suspect that this work will have broad utility in formulating design of optimal synthetic metabolic pathways.

## RECENT PUBLICATIONS


Kyle J. Tomek; Carlos Rafael Castillo Saldarriaga; Fernando Peregrino Cordoba Velasquez; Tongjun Liu; David B. Hodge; Timothy A. Whitehead. "Removal and upgrading of lignocellulosic fermentation inhibitors by in situ biocatalysis and liquid-liquid extraction," *Biotechnology and Bioengineering.* 2015;112(3):627–632. (2015)

Dahai Gao; Carolyn Haarmeyer; Venkatesh Balan; Timothy A. Whitehead; Bruce E Dale; Shishir P.S. Chundawat. "Lignin triggers irreversible cellulase loss during pretreated lignocellulosic biomass saccharification," *Biotechnology for Biofuels.* 2014;7(1). (2014)

Matthew S. Bienick; Katherine W. Young; Justin R. Klesmith; Emily E. Detwiler; Kyle J. Tomek; Timothy A. Whitehead. "The interrelationship between promoter strength, gene expression, and growth rate," *PLoS ONE.* 2014;9(10). (2014)

# R. Mark Worden

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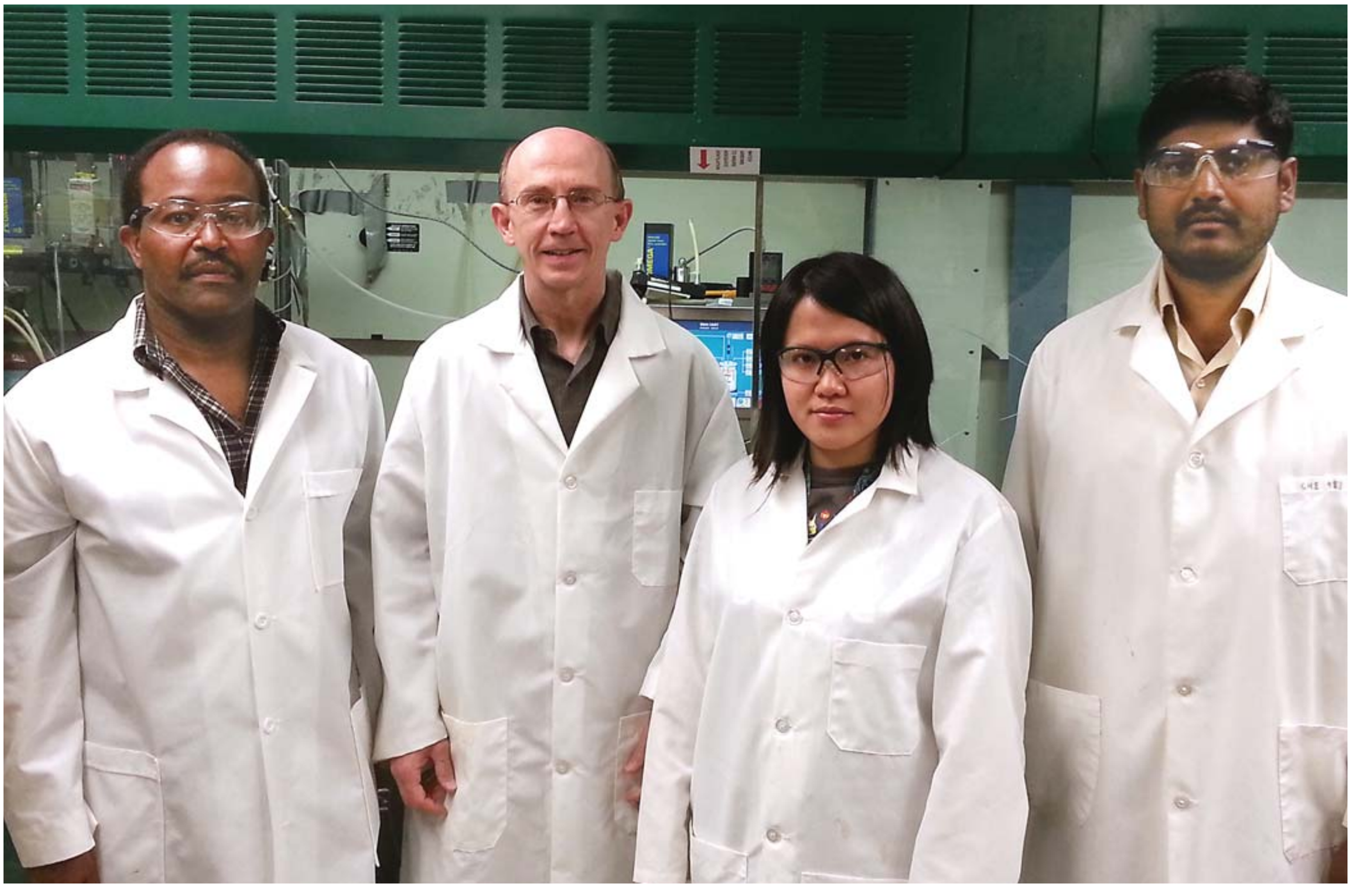

**FIGURE 1.** Worden's research group for the Department of Energy ARPA-E Electrofuels project. *Left to right:* Lee Alexander, Dr. Worden, Chloe Liu, and Soumen Maiti.

## RESEARCH INTERESTS

Multiphase biocatalysis, nanobiotechnology, biomimetic interfaces, biosensors, bioelectronics

## LAB & LOCATION

Nanobiotechnology and Biomimetic Interfaces, 428 S. Shaw Lane, Room 2525

## WEBSITE

http://www.chems.msu.edu/people/profile/worden?user=worden

## GROUP MEMBERS

Paul Sharpe, Kirti Bhardwaj, Serban Peteu

## RECENT PATENTS GRANTED (9 TOTAL)

Worden, R.M. et al. Nanostructured biosensor containing neuropathy target esterase activity. US Patent 8623196, January 7, 2014.

Worden, R.M. et al. Customizable and renewable nanostructured interface for bioelectronic applications. US Patent 8435773, May 7, 2013.

## CURRENT RESEARCH FOCUS

Dr. Worden's focus on multiphase biocatalysis 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 $H_2$, $CO_2$ and $O_2$ 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 $H_2$ and $O_2$ 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 $H_2$ and $O_2$ 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 $H_2$, $CO_2$, and $O_2$.

Dr. Worden's focus on nanobiotechnology and biomimetic interfaces 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 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.

Dr. Worden's focus on biosensors and bioelectronics 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 a 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" (7 co-Is) and "Multidisciplinary Graduate Training Program on Technologies for a Biobased Economy (7 co-Is). He also served as PI of a grant from the NSF Combined Research and Curriculum Development program to develop a novel "Multidisciplinary Bioprocessing Laboratory" course (5 co-PIs). He and a colleague from the Michigan Biotechnology Institute were funded by the U.S. State Department to co-develop a fermentation scale-up training program for Russian bioscientists entitled "Fermentation Pilot-Plant Training for Sibbiopharm Staff."

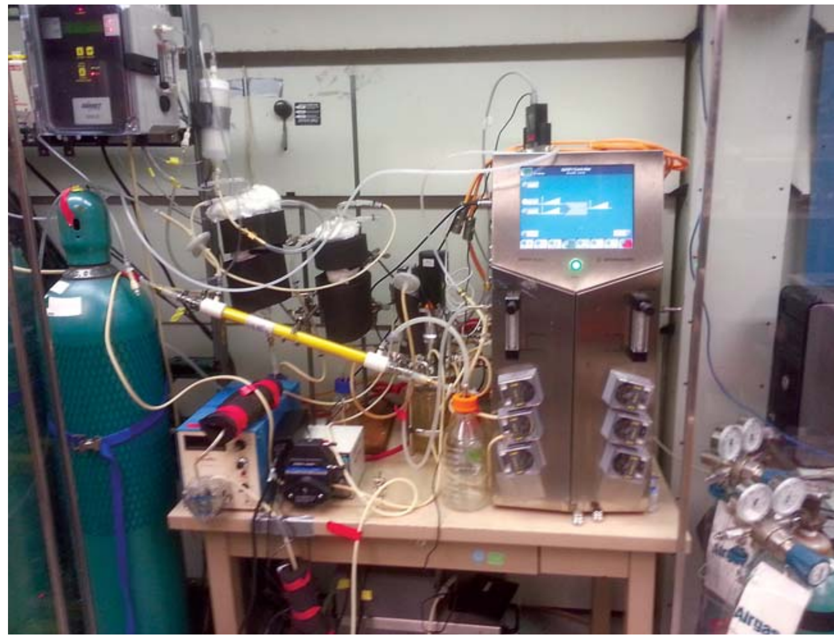

**FIGURE 2.** Photograph of prototype Bioreactor for Incompatible Gases (BIG) assembled in walk-in fume hood of Dr. Worden's laboratory.

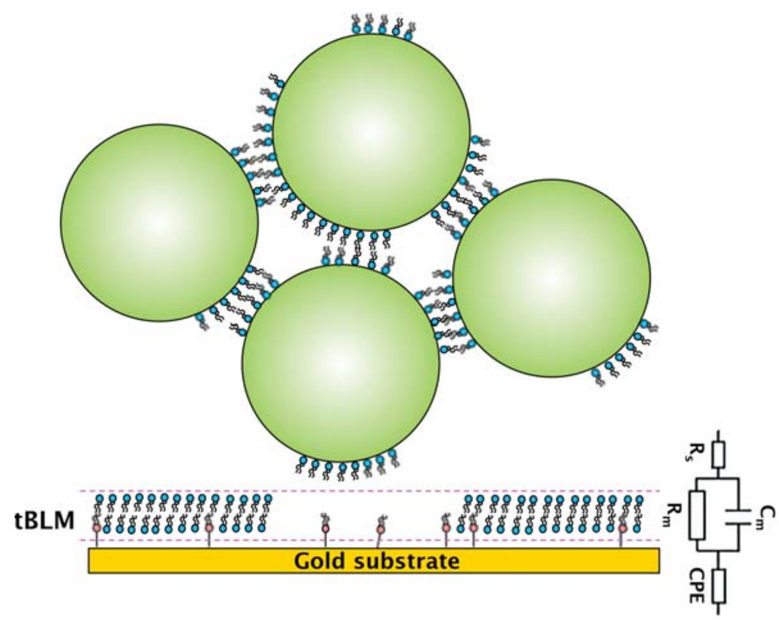


**FIGURE 3.** Schematic diagram of nanoparticles (spheres) removing lipid molecules from a biomembrane (shown as a layer of lipid molecules on the gold electrode).

## RECENT PUBLICATIONS

Hanzi Li; Rui Li; Robert M. Worden; Scott Calabrese Barton. "Facilitation of high-rate NADH electrocatalysis using electrochemically activated carbon materials," *ACS Applied Materials and Interfaces.* 2014;6(9):6687–6696. (2014)

Ying Liu; Zhen Zhang; Quanxuan Zhang; Gregory L. Baker; R. Mark Worden. "Biomembrane disruption by silica-core nanoparticles: Effect of surface functional group measured using a tethered bilayer lipid membrane," *Biochimica et Biophysica Acta–Biomembranes*. 2014;1838(1 PARTB):429–437. (2014)

Ying Liu; R. Mark Worden. "Size dependent disruption of tethered lipid bilayers by functionalized polystyrene nanoparticles," *Biochimica et Biophysica Acta–Biomembranes*. 2014;1848(PA):67–75. (2014)

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