
THE UNIVERSITY OF ALABAMA[®]



GRADUATE RESEARCH OPPORTUNITIES

2023/2024

THE UNIVERSITY OF
ALABAMA[®]

College of
Engineering
Chemical and Biological Engineering

Research Overview

Biomaterials and Biotechnology

BAO – BRAZEL – KIM – RAO – SUMMERS – ZHAO

Catalysis and Electrocatalysis

HARRIS – HUANG – RITCHIE – SHEEHAN – SUN – SZILVÁSI
TURNER – WANG

Computational/Thermodynamics

BARA – ESFAHANI – HENDERSON – SHEEHAN – SZILVÁSI –
TURNER

Electronic Materials and Devices

GUPTA – HENDERSON – HUANG – KLEIN – KOH

Energy/Environmental/Water

BARA – ESFAHANI – KOH – RITCHIE – SHEEHAN – WEINMAN

Membranes and Polymers

BARA – BRAZEL – ESFAHANI – HENDERSON – KOH – RITCHIE
WANG – WEINMAN – ZHAO

Graduate Coordinator

Dr. Yuping Bao, ybao@eng.ua.edu

FACULTY

Yuping Bao, Ph.D., Washington

Jason E. Bara, Ph.D., Colorado

Christopher S. Brazel, Ph.D., Purdue

Milad Esfahani, Ph.D., Tenn Tech

James W. Harris, Ph.D. Purdue

Clifford L. Henderson, Ph.D., UT-Austin

Qiang Huang, Ph.D., LSU

Yonghyun (John) Kim, Ph.D., UMBC

Tonya M. Klein, Ph.D., NC State

Amanda Koh, Ph.D., Rensselaer

Shreyas S. Rao, Ph.D., Ohio State

Stephen Ritchie, Ph.D., Kentucky

James Sheehan, Ph.D., Penn State

Ryan Summers, Ph.D., Iowa

H. (Harold) Hohyun Sun, Ph.D., UT-Austin

Tibor Szilvási, Ph.D., BME, Hungary

C. Heath Turner, Ph.D., NC State

Zhongyang Wang, Ph.D., Wash U St. Louis

Steven Weinman, Ph.D., Clemson

John M. Wiest, Ph.D., Wisconsin

Chao Zhao, Ph.D., Akron



Program Highlights

Innovation, Entrepreneurship, and Creating New Opportunities

Our students and faculty are constantly exploring new ideas, venturing into new areas, and looking for solutions to society's most pressing challenges. Translating a theoretical concept into a tangible product is one of the most exciting aspects of our research portfolio, often leading to a patent, a new business venture, or a licensing opportunity. *Did you know... Prof. Huang currently holds 43 U.S. patents!*

Faculty Leadership and Student Mentoring

We strive to create a challenging and supportive research environment for our students, by providing opportunities to work side-by-side with some of the most creative and intellectually-renown researchers in the world. With publications in top journals and some of the most prestigious academic awards in the world, our students and faculty work together as a team. *Did you know...our faculty may have already contributed to your education with their textbooks (Fundamental Principles of Polymeric Materials, Prof. Brazel; Separation Process Essentials, Prof. Lane) or mobile applications (Chemical Engineering App Suite for iPhone/iPad, Prof. Bara)!*

On-Campus Facilities and International Exposure

Our facilities have been transformed by a recent investment of \$240 million to create the Science and Engineering Quad, with modern labs, environmental sustainability, and access to state-of-the-art analytical characterization tools. Our capabilities are leveraged to form international partnerships and research collaboration opportunities for our students and faculty around the globe. *Did you know...our students regularly receive international research recognition, and our faculty have won some of the most prestigious international awards (Fulbright Distinguished Scholar, Profs. Brazel and Kim)!*

Tuscaloosa, AL: The University of Alabama is located in the heart of Tuscaloosa (<https://visittuscaloosa.com>), home to one of the most beautiful campuses in the nation, along with a very mild climate and a low cost of living. It is about a 4-hour drive to the gulf coast where you will find some of the most breathtaking beaches in the world (<https://www.gulfshores.com/>). Birmingham is the largest neighboring city (1-hour drive), with a population of approximately 1 million residents. If you need more information about The University of Alabama and life on our campus, please visit: <https://www.ua.edu/about/>



Research Support

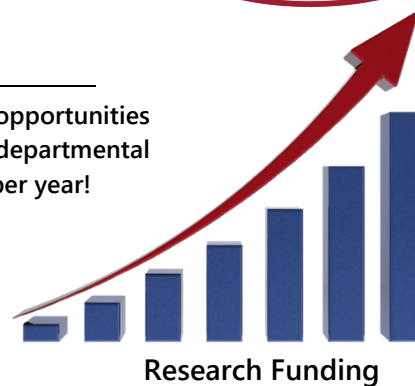
Funding the Best and Brightest Ideas

Approximately 30% of the faculty have received NSF-CAREER Awards (NSF's most prestigious award in support of early-career faculty), as well as other national recognition of research and teaching excellence.

Over 80% annual
growth rate!

A Period of Unprecedented Growth

Research funding has been growing at a rapid pace, creating new opportunities and increasing the impact of our work. Over the last five years, the departmental research funding has been growing at an average pace of over 80% per year!



Broad Research Support

Research projects are sponsored by a wide variety of state, regional, and federal agencies, as well as private companies. Whether you are interested in working with a federal agency, a private company, a government laboratory, or ultimately pursue a career in academics, we can help pave the way.



U.S. DEPARTMENT OF
ENERGY





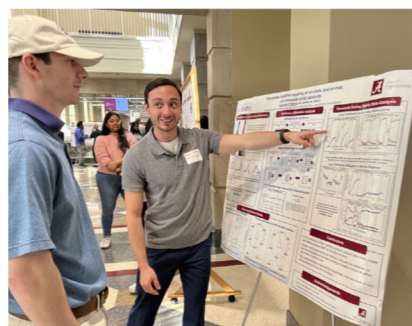
Professional Development

Networking Opportunities

Our research success is driven by passionate faculty, graduate students, and postdoctoral students, and we are all stronger together. Throughout the year, we provide multiple opportunities to connect and collaborate, including seminar visits from external distinguished researchers, Meet Your Neighbor lunches, our Annual ChBE Research Symposium, Peer Mentoring, and even an International Food Festival!

Presentation and Communication Experience

One of the most valuable skills in a research career is the ability to deliver a clear and impactful presentation. Our students are given frequent opportunities to participate in regional and on-campus events, as well as the ability to travel to national and international conference venues to present their research.



Outreach and Community Engagement

If you want to make a real impact in the lives of others, a graduate degree in chemical engineering can provide many opportunities. Our research projects extend far beyond the benchtop, including work with local schools, public utilities, and hands-on science museums.



Faculty Research Profiles

Yuping Bao

Nano-Bio Interface Laboratory - Multifunctional Nanostructures for Imaging-guided Drug delivery and Drug Discovery



Yuping Bao.

Associate Professor
Ph.D. Materials Science and
Engineering and Nanotech.
Univ. Washington, 2006

Recent Publications

Z. C. Arituluk, J. Horne, B. Adhikari, J. Steltzner, S. Mansur, P. Ahirwar, S. E. Velu, N. E. Gray, L. Ciesla, Y. Bao, Identification of TrkB Binders from Complex Matrices Using a Magnetic Drug Screening Nanoplatfrom, *ACS Applied Bio Materials* 4, 6244 (2021).

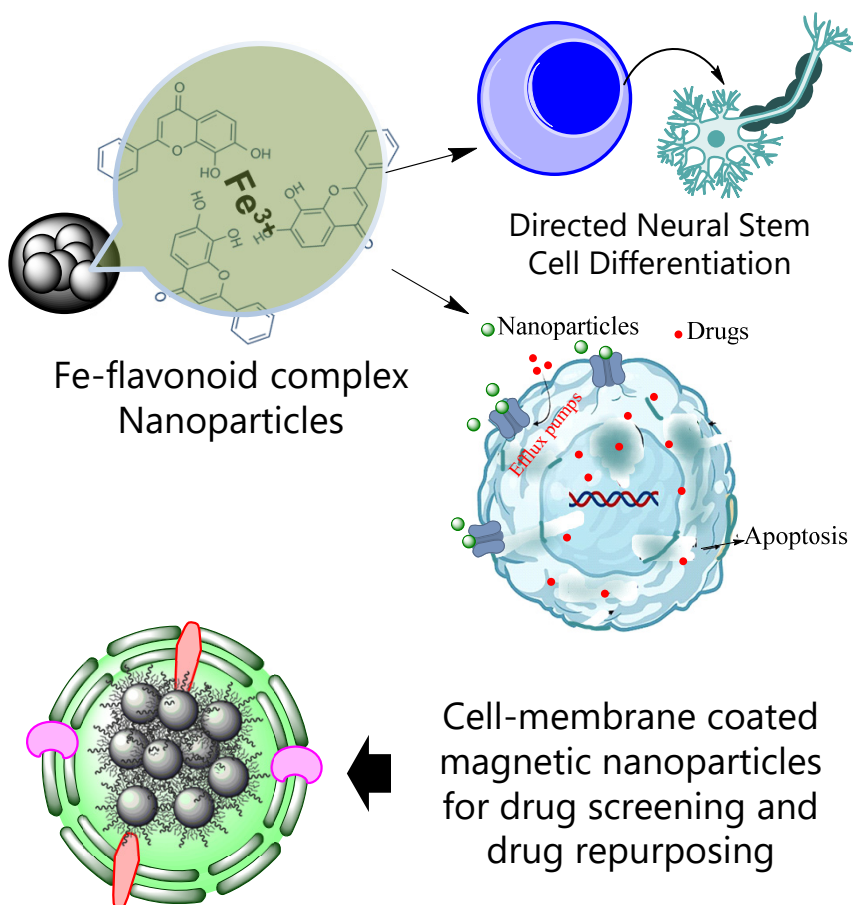
T. Barjesteh, S. Mansur, Y. Bao, Inorganic Nanoparticle-Loaded Exosomes for Biomedical Applications, *Molecules* 26, 1135 (2021).

J. Horne, S. Mansur, Y. Bao, Sodium Ion Channels as Potential Therapeutic Targets for Cancer Metastasis, *Drug Discovery Today* 26, 1136 (2021).

Dr. Bao's group focuses on designing novel multifunctional nanosystems for drug delivery and drug discovery.

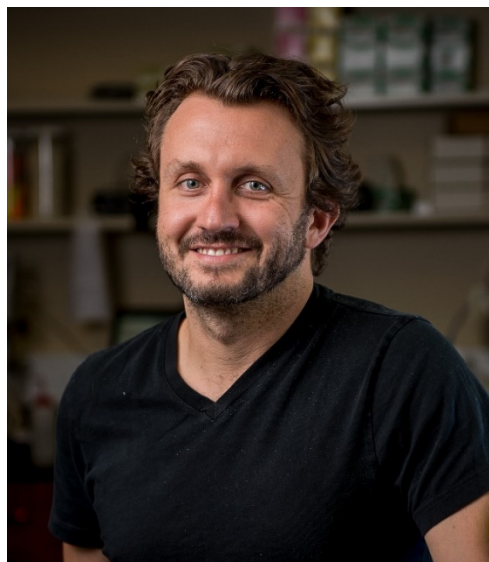
Much of Dr. Bao's work is related to the design of nanocarriers for targeted drug delivery, including multifunctional nanocarriers for overcoming drug resistance and directed stem cell differentiation. One of the unique aspects of the nanocarrier design is the use of natural products, such as flavonoids. In addition, the use of an Fe complex allows for MRI tracking.

The Bao group is also heavily working on the development of a drug screening platform for drug repurposing and new drug development. The designed drug screening platform has two distinct benefits: (1) screening against transmembrane receptors, and (2) ability to screen mixtures, eliminating the need to analyze each compound.



Jason E. Bara

Molecular Design of Advanced Polymers, Gas Separation Membranes, "Green" Chemistry, Ionic Liquids, 3D Printing, Polymer Upcycling and Depolymerization, Chemical Engineering Mobile Apps



Jason E. Bara

Professor

Ph.D. Chemical Engineering
University of Colorado at
Boulder, 2007

Recent Publications

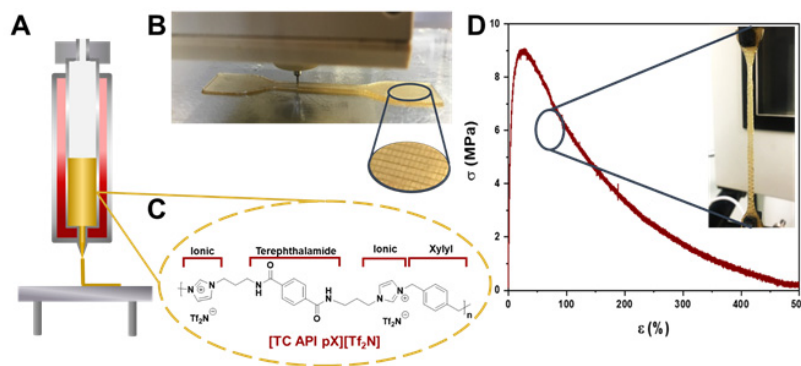
K. E. O'Harra, I. Kammakam, Y. Tuan, E. M. Jackson, J. E. Bara, PEEK-Ionenes: Ultrahigh-Performance Polymers Meet Ionic Liquids, *ACS Appl. Polym. Mater.* 4, 8365 (2022).

I. Kammakam, K. E. O'Harra, J. E. Bara, E.M.Jackson, Spirobisindane-Containing Imidazolium Polyimide-Ionene: Structural Design and Gas Separation Performance of "Ionic PIMs", *Macromolecules* 55, 4790 (2022)

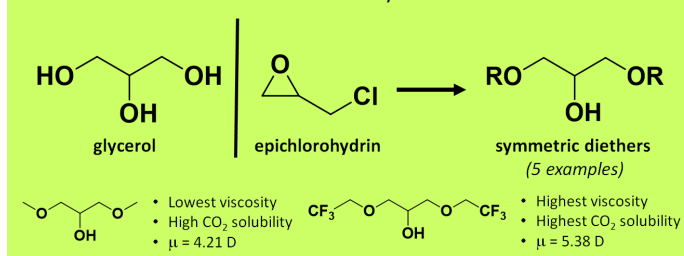
Dr. Bara's research group is focused on upcycling and depolymerization of plastic wastes; molecular design of membranes, sorbents and solvents; green chemicals; 3D printing of self-healing and stimuli-responsive polymers; scientific and educational apps for iPhones and iPads.

Dr. Bara is a recognized leader in the molecular design of polymers and composites, especially those based on ionic liquids and imidazoles. The highly tunable chemical and physical properties of these materials enable applications including gas separation membranes; superabsorbent materials for organic solvents; and stimuli-responsive, shape-memory, and self-healing polymers that can be 3D printed. Dr. Bara's group is also very active in the synthesis and study of new "green" solvents derived from glycerol. He is also pioneering research in plastic waste upcycling and depolymerization, with a particular emphasis on PVC.

3D Printing of Self-Healing Polyamide-Ionene



Green Solvents with Glycerol Skeletons



Christopher Brazel

Toxicological Evaluation of Novel Materials, Polymers, Magnetic Hyperthermia, Nanotherapeutics, Single-use Bioprocessing Films



Christopher Brazel

Associate Professor
Ph.D. Chemical Engineering
Purdue University, 1997.

Recent Publications

Shah, R.R., T.W. Linville, A. Whynot and **C.S. Brazel**, "Evaluating the toxicity of bDtBPP on CHO-K1 cells for testing of single-use bioprocessing systems considering media selection, cell culture volume, mixing, and exposure duration," *Biotech. Progress* 32, 1318-1323 (2016).

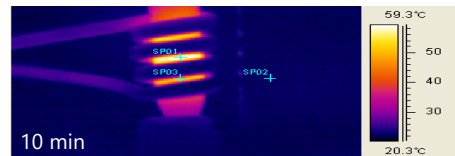
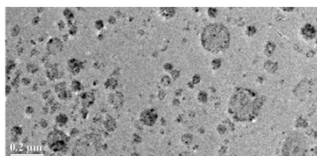
R.R. Shah, A.R. Dombrowsky, A.L. Paulson, M.P. Johnson, D.E. Nikles, and **C.S. Brazel**, "Determining iron oxide nanoparticle heating efficiency and elucidating local nanoparticle temperature for application in agarose gel-based tumor model," *Mater. Sci. Eng. C* 68, 18-29 (2016).

The Brazel Laboratory is interested in developing and understanding the chemical and biological properties of materials for medical, biopharmaceutical, and chemical processing applications. Recent foci in the lab include: (1) developing a robust toxicology assay to evaluate polymer films for single-use cell culture/fermentation as well as ionic liquids used in recycling of materials, and (2) development of targeted magnetic micelles that combine hyperthermia with drug release for cancer therapy.

We seek to understand the fundamental chemistry and physics of the materials and phenomena to guide the optimization of materials used in bio- and chemical-processing and drug delivery devices, while considering the interaction of new materials with both the human body (therapeutic effect) and the environment (potential toxicology).

In the area of toxicology, the biopharmaceutical industry is growing ever-more dependent on single-use plastics for sterile, off-the shelf solutions to growing cells. With this comes the potential exposure of cells used to manufacture complex medicines to plastics additives that may impair cell growth or lead to unsafe by-products. By developing toxicological assays, standardized tests can be developed to compare products made across the industry and safer plastics developed to ensure high quality production.

In the area targeted magnetic micelles, the combination of nanoparticles with polymeric micelles allows a magnetic field to trigger release of chemotherapy agents. Our lab includes synthesis of iron oxide nanoparticles, self-assembly of poly(caprolactone-b-ethylene glycol) block copolymers and characterization of the properties and functionality of these materials. Electron microscopy (TEM image of magnetic micelles below, left), and high frequency magnetic heating (envisioned using an infrared camera, bottom right) are used to validate the system.



Milad Rabbani Esfahani

Functionalized Membranes for Water Purification & Desalination, Metal Organic Framework, Adsorption, Wastewater Treatment



Milad R. Esfahani

Assistant Professor
Ph.D. Chemical Engineering
Tenn. Tech. University, 2015

Recent Publications

M. Kasula, T. Le, A. Thomsen, **M. R. Esfahani**, Silver metal organic frameworks and copper metal organic frameworks immobilized on graphene oxide for enhanced adsorption in water treatment, *Chemical Engineering Journal* 439, 135542 (2022).

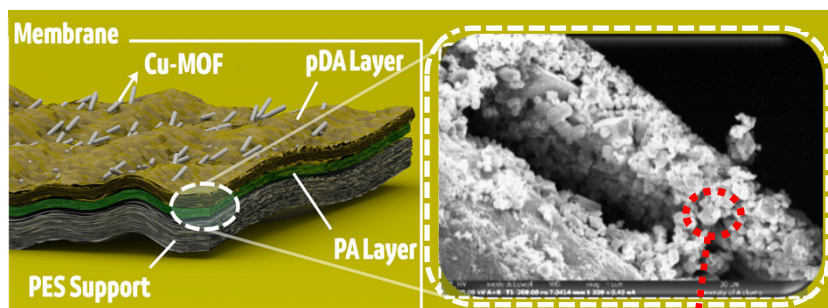
T. Le, E. Jamshidi, M. Beidaghi, **M. R. Esfahani**, Functionalized-MXene Thin-Film Nanocomposite Hollow Fiber Membranes for Enhanced PFAS Removal from Water, *ACS Applied Materials & Interfaces* 14, 22, 25397 (2022).

Dr. Esfahani's group uses a multidisciplinary approach to develop novel functionalized membranes and metal organic frameworks (MOFs) with the ultimate goal of water and wastewater treatment.

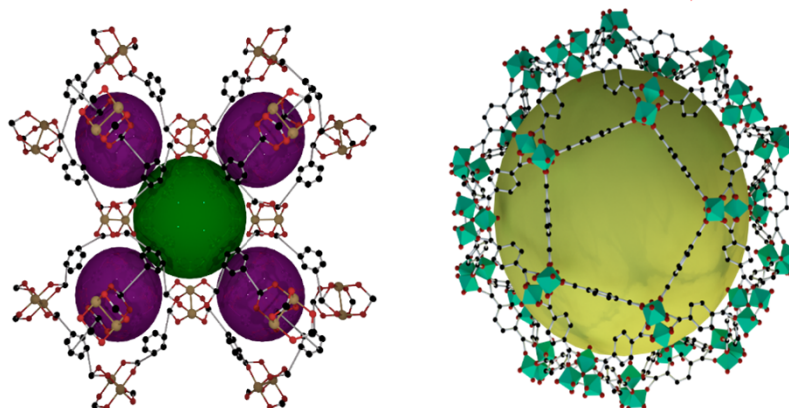
The Esfahani Research Group focuses on membrane functionalization and synthesizing novel adsorbents for water/wastewater treatment and desalination.

We develop strategies to functionalize different polymeric membranes, including thin-film composite nanofiltration and reverse osmosis membranes, for enhanced selectivity, permeability, and antifouling. Esfahani Research Group synthesizes a variety of metal organic frameworks (MOFs) as the new adsorbents or develops MOF-functionalized membranes for the selective removal of emerging contaminants such as PFAS and micro-nano plastics from water.

MOF- Functionalized Membrane



Metal Organic Frameworks



James W. Harris

Synthesis and Characterization of Inorganic Solids, *In Situ* Spectroscopy, Chemical Reaction Engineering, Chemical Kinetics



James W. Harris

Assistant Professor
Ph.D. Chemical Engineering
Purdue University, 2017

Recent Publications

J. W. Harris, J. S. Bates, B. C. Bukowski, J. Greeley, and R. Gounder, Opportunities in Catalysis Over Metal-Zeotypes Enabled by Descriptions of Active Centers Beyond Their Binding Sites, *ACS Catal.* 10, 9476 (2020)

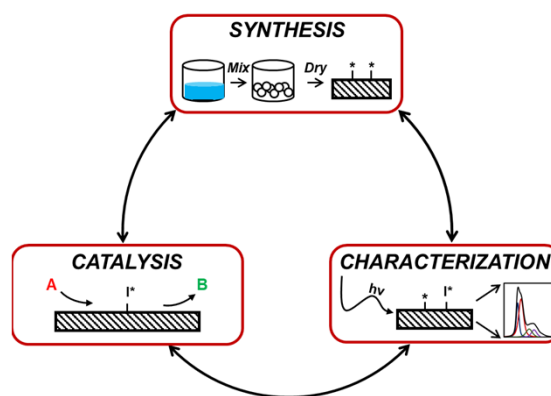
J. W. Harris, A. V. Verma, J. A. Arvay, A. J. Shih, W. N. Delgass, and F. H. Ribeiro, Consequences of Product Inhibition in the Quantification of Kinetic Parameters, *J. Catal.* 389, 468 (2020)

J. W. Harris, and A. Bhan, Kinetics of Chlorine Deposition and Removal over Promoted Silver Catalysts During Ethylene Epoxidation, *J. Catal.* 380, 318 (2019)

Dr. Harris's group studies chemical reactions occurring at solid surfaces in order to develop environmentally friendly catalytic routes to fuels and chemicals.

Catalysts provide energetically feasible pathways for chemical reactions to occur. The Harris group works to understand these materials as they exist during reaction in order to develop processes to upgrade abundant feedstocks to desirable chemicals. We synthesize catalysts, including supported metal nanoparticles and crystalline microporous solids, and characterize their physical and chemical characteristics at the molecular level. These materials are used for studies of the kinetics and mechanisms of chemical reactions, with aid from *in situ* spectroscopic tools, to develop improved processes that reduce the environmental impacts of the production of fuels and chemicals.

Research in our group includes efforts to transform shale gas to useful chemicals. Abundant reserves of shale gas in the United States have provided a surplus of light alkanes and provided an opportunity to develop new catalytic processes to transform these feedstocks into useful chemicals and fuels instead of flaring these gases at geographically isolated shale gas wells. Emerging classes of catalysts have demonstrated exciting prospects for the selective transformation of these light alkanes into liquid chemicals that are more easily transported.



A second area of research involves upgrading of oxygenates derived from biomass. These highly-functionalized molecules can act as platform molecules for production of fuels, polymer precursors, solvents, flavorings, perfumes, and pharmaceutical precursors. Production of these high-value chemicals currently requires non-renewable feedstocks and often generates toxic by-products, leading to opportunities to explore selective catalytic transformations that alleviate existing environmental impacts while producing renewable specialty chemicals.

Clifford L. Henderson

Functional Polymers and Organic Nanotechnology Lab



Clifford L. Henderson

Dean and Professor
Ph.D. Chemical Engineering
University of Texas Austin,
1998

Recent Publications

J.B. Delony, P.J. Ludovice, and **C. L. Henderson**, Block copolymer directed self-assembly defect modes induced by localized errors in chemoepitaxial guiding under layers: A molecular simulation study. *J. Vac. Sci. Technol. B* 38, 032604 (2020).

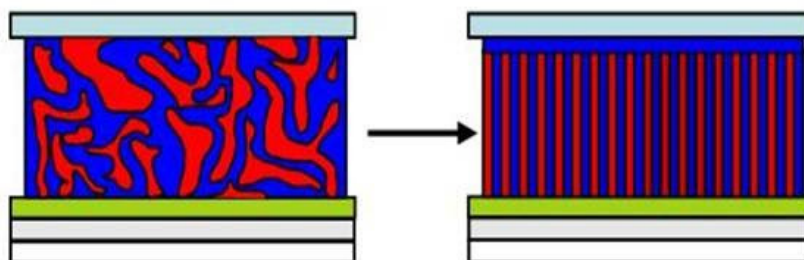
B. L. Sharp, H. L. Narcross, P. Ludovice, L. M. Tolbert, **C. L. Henderson**, Structural effects on the performance of epoxide-based negative-tone molecular resists. *J. Vac. Sci. Technol. B* 37, 011604 (2019).

Dr. Henderson's work intersects a variety of topics including polymer science, thin film science and technology, organic chemistry, nanoscience & nanotechnology, nanomanufacturing, molecular modeling and molecular dynamics, and electronic and optical materials and devices.

Our research focus broadly lies at the intersection of chemical engineering, chemistry, and materials science, where in many cases the general goals of our work are: (1) to understand the connections between chemical structure, material processing, and properties in advanced materials, (2) to develop materials and processes that allow for high definition patterning of materials and formation of nanostructured materials that enhance their function, and (3) to use these materials and processes to fabricate novel devices and structures for a variety of applications.

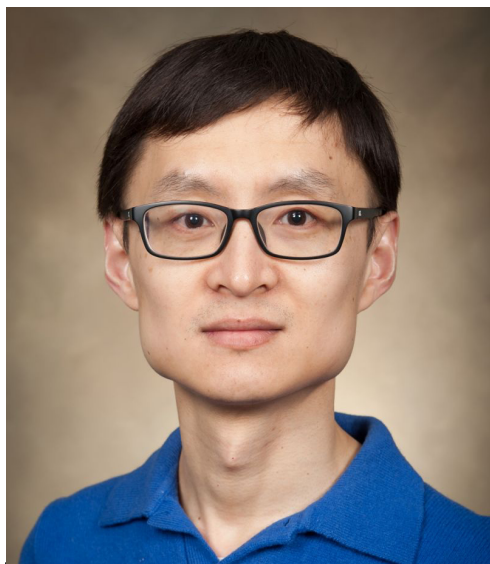
Examples of current projects include: (1) design of new block copolymers and processes for the directed self assembly (DSA) and fabrication of nanostructures, (2) modeling and simulation of block copolymer phase separation using advanced and novel molecular dynamics techniques, (3) design of new photoresist materials and processes for sub-20nm patterning, (4) studies of the physicochemical property behavior of polymer ultra-thin films, and (5) directed synthesis of graphene.

Organic Photovoltaic (OPV) systems are being engineering to capture sunlight more efficiently by using block copolymers to produce ordered materials with feature length scales commensurate with exciton charge pair separation distances.



Qiang Huang

Electrochemical Engineering for Nanomaterials, Nanostructures and Nanodevices



Qiang Huang

Associate Professor
Ph.D. Chemical Engineering
Louisiana State University, 2004

Recent Publications

Y. Hu, and **Q. Huang**, Oscillatory Behavior in Cobalt Electrodeposition with 3-Mercapto-1-Propanesulfonate, *J. Phys. Chem.*124, 21608 (2020).

W. Sides, E. Hassani, D. Pappas, T. Oh, and **Q. Huang**, Grain Growth and Superconductivity of Rhenium Electrodeposited from Water-in-Salt Electrolytes, *J. Appl. Phys.*127, 085301 (2020).

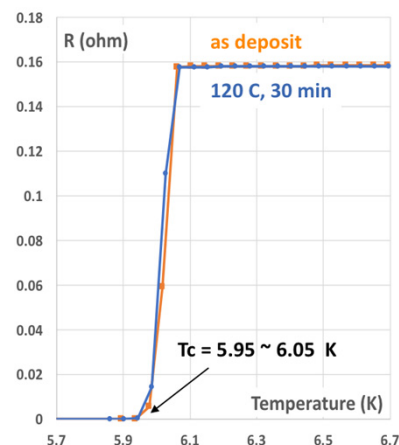
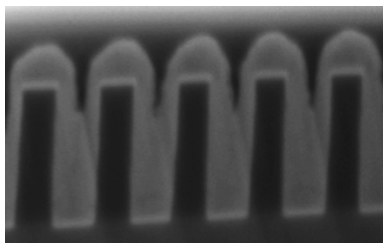
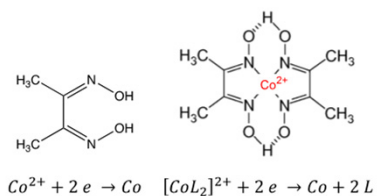
S. De, J. White, T. Brusuelas, C. Patton, A. Koh, and **Q. Huang**, Electrochemical Behavior of Protons and Cupric Ions in Water in Salt Electrolytes with Alkaline Metal Chloride, *Electrochim. Acta.* 228, 135852 (2020).

Dr. Huang's group focuses on developing electrochemical technologies to fabricate new materials and structures for applications in microelectronics, renewable energy, and quantum devices.

Electrochemical reactions are chemical reactions that involve electron transfer. Dr. Huang's current research focuses on such reactions in conjunction with materials sciences, investigating the impacts of the chemistry and process on the material structure and properties. Two example applications are for microelectronic and quantum devices.

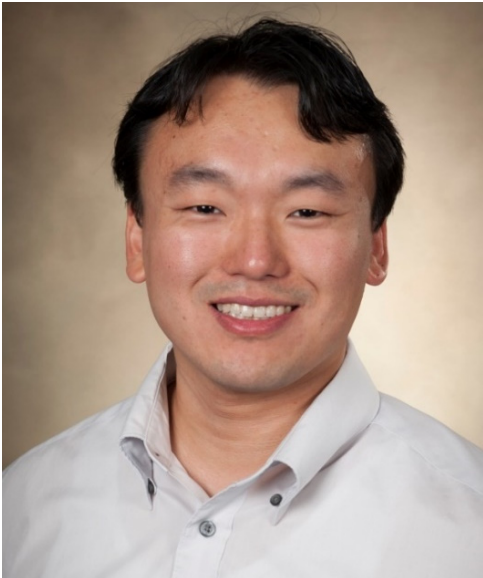
The convenience of our daily life and the development of modern technology heavily rely on the advancement of microelectronic and semiconductor devices. Interconnect is a nanometer sized network of metal wires in integrated circuits, enabling the communication between each semiconductor devices (transistors). We are exploring the electrochemistry and electrodeposition process for the fabrication of new interconnects, which are much needed to enable the further advancement of integrated circuits, as well as our computers and cell phones. (Figure on the left)

Quantum computing is believed to represent a completely new paradigm, where the data are no longer zeros and ones but rather can be any values in between. We are developing new electrochemical methods to make superconducting films and superconductor-based quantum junction devices. Such films allow the passage of electrons without any resistance, avoiding electrical heating and temperature perturbation on the cryogenic quantum computer. (Figure on the right)



Yonghyun (John) Kim

Bioengineering, Oncology, Translational Medicine



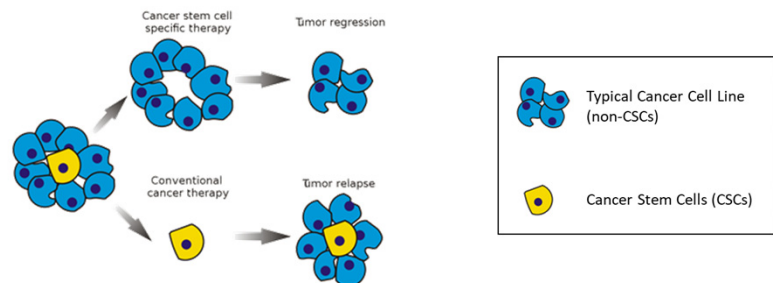
Yonghyun (John) Kim
Associate Professor
Ph.D. Chemical Engineering
Univ. Maryland Baltimore
County, 2008

Recent Publications

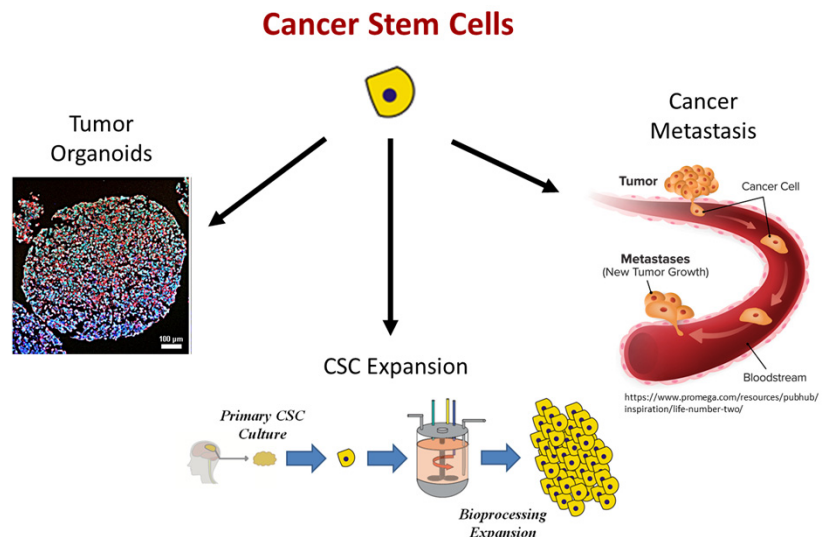
S. Park, A. D. Avera, Y. Kim, Biomanufacturing of Glioblastoma Organoids Exhibiting Hierarchical and Spatially Organized Tumor Microenvironment via Transdifferentiation, *Biotechnol Bioeng.*, doi: 10.1002/bit.28191 (2022).

S. R. Brown, J. C. Bates, A. D. Avera, Y. Kim, Relationship Between Stemness, Reactive Oxygen Species, and Epithelial-to-Mesenchymal Transition in Model Circulating Tumor Cells, *Cells Tissues Organs* 211, 282 (2022).

The Kim laboratory is working on bioengineering of cancer stem cells (CSCs) to better assist translational medicine.



CSCs are the stem cell-like pluripotent cancer cells that cause relapse in patients even after the most rigorous treatment. Pharmaceutical companies typically use several decades-old cancer cell lines during their drug development because, among many reasons, (1) CSCs are difficult to acquire and (2) are limited in number. It is becoming increasingly recognized, however, drug development must be based on CSCs to develop better drugs that target the "real culprit" in tumors. Therefore, the work at the Kim Laboratory aims to bridge the oncologists with the engineers by developing various bioengineering models that better recapitulate patient tissues using CSCs. By doing so, we hope to assist in the drug development by providing a more relevant and closer-to-clinic resource of cancer cells. Recent efforts include the development of **brain tumor organoids** and fluid shear stress-based **breast cancer metastatic models**.



Tonya Klein

In-situ IR Spectroscopy of Thin Film Deposition



Tonya Klein

Associate Professor
Ph.D. Chemical Engineering
North Carolina State
University, 1999

Recent Publications

Z. Fang, M. P. Confer, Y. W. Wang, Q. Wang, M. Ross Kunz, E. J. Dufek, B. Liaw, **T. M. Klein**, D. A. Dixon, R. Fushimi, Formation of Surface Impurities on Lithium-Nickel-Manganese-Cobalt Oxides in the Presence of CO₂ and H₂O *Journal of the American Chemical Society* 143, 10261 (2021).

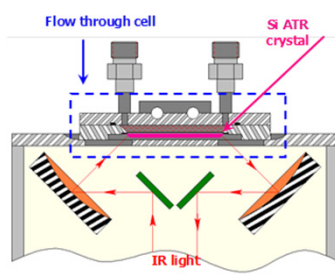
M. P. Confer, A. DeSimone, H. Burnham, W. McLeod, **T. M. Klein**, S. C. Street, D. A. Dixon, Solubility thermodynamics of amine boranes in polar solvents, *International Journal of Hydrogen Energy* 4610801 (2021).

Material interfaces affect performance of electronic, magnetic and photonic devices presenting an ever-pressing need to characterize the physics and chemistry of solid surfaces. Technologies such as spin valves, field effect transistors, and nano-laminate optical coatings are comprised of ultra-thin films in the nanometer thickness regime.

At this dimension, bulk thermodynamic properties governing film stability, diffusion, and reactions as well as bulk electron transport mechanisms that determine device performance no longer apply. Hence, there is a need to develop novel preparation procedures for thin film structures with abrupt interfaces for incorporation in new devices and in test devices which probe fundamental physical phenomena like electron scattering at interfaces in giant magneto resistance (GMR) and tunneling magneto resistance (TMR) recording heads.

Atomic Layer Chemical Vapor Deposition is a promising technique for the fabrication of nanometer scale thin films for alternate high k gate dielectrics in field effect transistors, dielectrics for magnetic tunnel junctions, and metal thin films for spin valves, optical coatings, or diffusion barriers for interconnects. The process involves a separation of the reaction sequence into two self-limiting steps dependent on the availability of functional groups present on the surface. This allows the formation of an atomic layer one step at a time, resulting in excellent film uniformity, conformality and thickness control.

Attenuated total reflectance Fourier transform infra-red spectroscopy (ATR-FTIR) reaction cell is used to observe initial reaction pathways in real time. An IR light beam is focused on the backside of a heated Si, Ge or ZnSe ATR crystal and is bounced though as it is totally reflected at the gas surface interfaces. Some of the light extends as an evanescent wave into the reaction zone on the topside of the ATR crystal and is used to identify key chemical groups involved in the reaction sequence.



Amanda Koh

Functional Material Interfaces for Soft Robotics, Stretchable Electronics, Sensing, and Environmental Remediation



Amanda Koh

Assistant Professor
Ph.D. Chemical Engineering
Rensselaer Polytechnic
Institute, 2016

Recent Publications

E. Bury, **A. S. Koh**, Multimodal Deformation of Liquid Metal Multimaterial Composites as Stretchable, Dielectric Materials for Capacitive Pressure Sensing, *ACS Appl. Mater. Interfaces* 14, 13678 (2022)

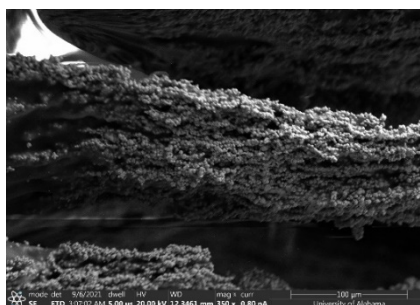
E. Bury, S. Thiagarajan, N. Lazarus, **A. S. Koh**, Ferrofluid High Internal Phase Emulsion Polymer Foams for Soft, Magnetic Materials, *J. Magn. Magn. Mater.* 563, 169921 (2022).

S. Thiagarajan et al., Study of n-Alkanethiol Self-Assembly Behavior on Iron Particles: Effect of Alkyl Chain Length and Adsorption Solvent on Resulting Iron-Based Magnetorheological Fluids, *Langmuir*, 38, 13506 (2022).

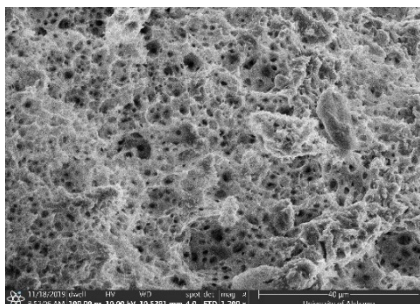
Dr. Koh's group focuses on engineering multifunctional materials through the intentional design of interfaces. Current research focuses on materials for soft robotics, stretchable electronics, smart materials, and environmental remediation.

As devices become more advanced in the fields of defense, health, and manufacturing, it is no longer enough for materials to have a single function or be useful to only a single application. Materials that are responsive and multifunctional are key to creating robust, practical, and adaptive systems. The Koh lab seeks to develop these materials through the engineering of internal and composite interfaces either through the manipulation of existing chemistry or the addition of novel components.

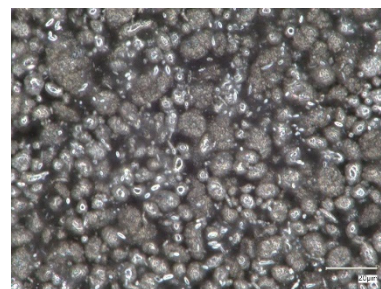
Much of the current work in Dr. Koh's lab focuses on developing soft materials which are both deformable and have electronic, magnetic, or sensing capabilities. Applications of these materials include stretchable electronics (ex. wearables and health monitoring), soft robotics (ex. human-machine interfaces and manned-unmanned teaming), and environmental contaminant remediation and sensing (ex. Harmful algal bloom toxins, chemical warfare agents, plastic byproducts).



Magnetically aligned magnetorheological fluid chain



High internal phase emulsion polymer foam



Liquid metal in PDMS dielectric dispersions

Shreyas Rao

Biomaterials, Cell-Material Interactions, Tumor Microenvironment, Drug Resistance



Shreyas Rao

Associate Professor
Ph.D., Chemical Engineering
The Ohio State University, 2012

Recent Publications

R. Kondapaneni, **S. S. Rao**. Matrix stiffness and cluster size collectively regulate dormancy versus proliferation in brain metastatic breast cancer cell clusters. *Biomater. Sci.* 8 (23): 6637-6646 (2020).

A. A. Narkhede, J. H. Crenshaw, D. K. Crossman, L. A. Shevde, **S. S. Rao**. An *in vitro* hyaluronic acid hydrogel based platform to model dormancy in brain metastatic breast cancer cells. *Acta Biomater.* 107,65 (2020).

P. S. Nakod, Y. Kim, **S. S. Rao**, Three-dimensional biomimetic hyaluronic acid hydrogels to investigate glioblastoma stem cell behaviors. *Biotechnol. Bioeng.* 117,511 (2020).

The Rao Laboratory is developing engineering tools to unravel the mechanisms associated with the role of microenvironment in cancer progression, therapeutic response and resistance.

The oncogenic progression of cancer from the primary to the metastatic setting is the critical event that defines stage IV disease, no longer considered curable. Despite some success in developing a suite of therapies, a key challenge that continues to hamper cancer treatment is the frequent development of drug resistance, particularly in the metastatic setting, resulting in disease relapse and often mortality. Most existing experimental models to investigate tumor cell responses to therapeutic treatments and examine mechanisms of drug resistance utilize two dimensional (2D) substrates (e.g., plastic, glass) that largely fail to recapitulate the complex *in vivo* environment.

Our research group is designing three dimensional (3D) biomaterial scaffolds (e.g., hydrogel scaffolds, and porous scaffolds) as tools to mimic features of tissues that could serve as platforms for elucidating physiologically relevant cellular behaviors, drug screening and discovery, as well as mechanisms of drug resistance in the context of cancer therapeutics *in vitro* and *in vivo*. In addition, we are developing biomaterial tools that could be employed for sensing and modulation of drug resistance. We are also applying systems biology approaches to understand the underlying mechanisms of therapeutic resistance in physiologically relevant 3D microenvironments. This knowledge could be subsequently utilized to devise strategies that can reprogram the microenvironment to halt disease progression. Given that drug resistance is a major issue noted across multiple types of cancers, this work would have far reaching implications in drug discovery and development, thereby transforming current treatment strategies.

Stephen Ritchie

Functionalized Materials for Separations, Catalysis, and Solid-phase Antimicrobials



Stephen Ritchie

Associate Professor
Ph.D. Chemical Engineering
University of Kentucky, 2001

Recent Publications

M. I. Hossain, A. Udoh, B. E. Grabicka, K. S. Walton, **S. M. C. Ritchie**, T. G. Glover, Membrane-Coated UiO-66 MOF Adsorbents, *Industrial & Engineering Chemistry Research* 58, 1352 (2019).

S. M. C. Ritchie, M. Costa-Teixeira, M., and R. M. Summers, Functional Surfaces in Food Processing, *Chemical Engineering Progress*, 52-55, (May 2019).

Dr. Ritchie's laboratory focuses on the addition of active properties to passive materials. This work has resulted in adsorptive membranes for antibody purification, highly charged membranes for protein separation and concentration, membrane catalysts, and anti-microbial surfaces. Commercial production of functionalized membranes and scale-up are also of interest.

The group's interest in adsorptive membranes has been focused on antibody purification. The work is continuing and evolving to include other biomolecules and more complex adsorption sites. Adsorptive membranes are fully synthetic and high capacity, and are capable of achieving similar selectivity to affinity resins.

We also have a strong interest in commercial production techniques and applications for functionalized membranes. Currently, work is focused on high volume systems containing proteins and other biomolecules. The goal is to concentrate proteins similar to conventional microfiltration and ultrafiltration processes, but at much higher flux through a combination of separation mechanisms beyond size exclusion.

The group's interest in acid catalysis has been on low temperature reactions where the competing solid-phase catalyst is strong acid ion exchange resin. Our current interest is adapting membranes for long-term operation in industrial systems. We are targeting applications with reactive distillation is currently employed.

We have also been active in synthesis of anti-microbial materials for application to dairy systems. Components of spiral-wound membrane elements can be modified to include anti-microbial surfaces. The particular application of interest is for *Listeria Monocytogenes* reduction in milk processing.

We have a new area of research on particle separation using non-woven materials formed from recycled plastics. Our focus will be on synthesis of fibers used in the application, as well as construction of composite materials that can provide similar performance to commercial filters applied to indoor air filtration.

James D. Sheehan

Chemical Valorization of Biomass and Waste Plastics, Reaction Engineering of Thermocatalytic Process, Reaction Kinetic Modeling



James D. Sheehan

Assistant Professor
Ph.D. Chemical Engineering
Pennsylvania State University,
2019

Recent Publications

J. D. Sheehan, E. Ebikade, D. G. Vlachos, and R. F. Lobo, Lignin-Based Water-Soluble Polymers Exhibiting Biodegradability and Activity as Flocculating Agents. *ACS Sustainable Chem. Eng.*, 10, 11117 (2022).

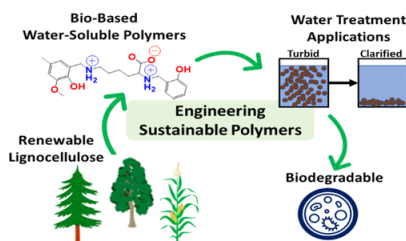
J. D. Sheehan, A. Abraham, and P. E. Savage, Reaction Pathways and Kinetics for Tetra-Alanine in Hot, Compressed Liquid Water. *React. Chem. Eng.* 4, 1237 (2019).

Dr. Sheehan's group uses experimental and modeling approaches to evaluate reaction kinetics and transport phenomena governing the chemical deconstruction of biomass and waste feedstocks. Their research develops sustainable processes for synthesizing commodity and fine chemicals.

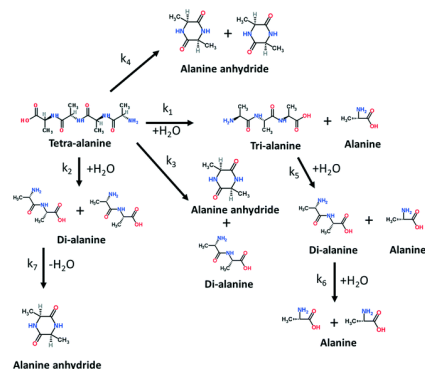
The research objective of the Sheehan group is to develop reactive processes that valorize abundant molecular feedstocks into value-added chemicals and support the expansion of a sustainable, chemical economy. To this end, the Sheehan Group investigates the reaction engineering of processes that valorize renewable and waste feedstocks (e.g., lignocellulosic biomass, organic waste, plastics) into value-added chemicals and materials. Investigations focus on evaluating thermochemical, catalytic, and supercritical fluid processes to chemically deconstruct and fractionate macromolecular feedstocks into small molecules. A combination of experimental and computational modeling tools are applied to evaluate the underlying transport phenomena and reaction kinetics governing these chemical fractionation processes.

Research Examples

Catalytic Fractionation of Biomass Deconstruction and Derivatization of Lignins into Eco-friendly Polymers



Chemical Kinetics Base-Catalyzed Hydrolysis of Peptides in Hot, Compressed Water



Ryan M. Summers

Metabolic Engineering, Synthetic Biology, Biochemical Engineering
for Production of Chemicals, Fuels, and Pharmaceuticals



Ryan Summers

Assistant Professor
Ph.D. Chem. and Bio. Engr.
University of Iowa, 2011.

Recent Publications

R. M. Summers, S. Gophishetty, S. K. Mohanty, and M. Subramanian, New Genetic Insights to Consider Coffee Waste as Feedstock for Fuel, Feed, and Chemicals, *Central Eur. J. Chem.* 12, 1271 (2014).

R. M. Summers, J. L. Seffernick, E. Quandt, C. L. Yu, J. Barrick, and M. Subramanian, Caffeine Junkie: An Unprecedented GST-Dependent Oxygenase Required for Caffeine Degradation by *P. putida* CBB5, *J. Bacteriol.* 195, 3933 (2013).

The Summers lab is working to metabolically engineer bacteria and yeast cells to produce chemicals, fuels, and pharmaceuticals. Specifically, the group focuses on engineering enzymes, gene networks, and genetic regulatory elements in microbial cells.

Caffeine is a natural product produced by many plants and consumed by humans worldwide. However, high caffeine consumption has also led to large amounts of caffeinated waste from coffee and tea processing plants. This can have detrimental environmental effects, as caffeine is toxic to most bacteria and insects. The Summers lab has a growing collection of bacteria capable of growing on caffeine as sole carbon and nitrogen source. From these bacteria, new genes and enzymes are being discovered that can be used in a variety of biotechnological applications. Through a combination of systems biology, protein engineering, and molecular biology, the lab is engineering yeast to simultaneously decaffeinate coffee waste and ferment the sugars in the waste to ethanol. Additionally, bacterial strains to produce high-value chemicals from caffeine are being created. The group is also working to determine the structures of caffeine-degrading enzymes in bacteria using X-ray crystallography.

Other projects in the Summers lab include metabolic engineering of probiotic bacteria for *in situ* delivery of amino acids, characterization of genetic regulatory elements in probiotic bacteria, design of modular plasmids for metabolic engineering of *E. coli*, *Saccharomyces cerevisiae*, and other microbial strains, and construction of novel riboswitches that recognize small molecules.

As society moves away from use of petroleum resources for production of fuels and chemicals, their replacements must come from natural, renewable resources. To meet this need, the Summers lab seeks to engineer bacteria and yeast cells to produce bulk and fine chemicals from biomass. In addition to these chemicals, the group is looking at production of pharmaceuticals and nutraceuticals in metabolically engineered microbial cells.

H. Hohyun Sun

Battery Materials for Electric Transport, Co-precipitation Reactions, Layered Oxide Cathodes, Functional Electrolytes



H. Hohyun Sun

Assistant Professor
Ph.D. The University of
Texas at Austin, 2020

Recent Publications

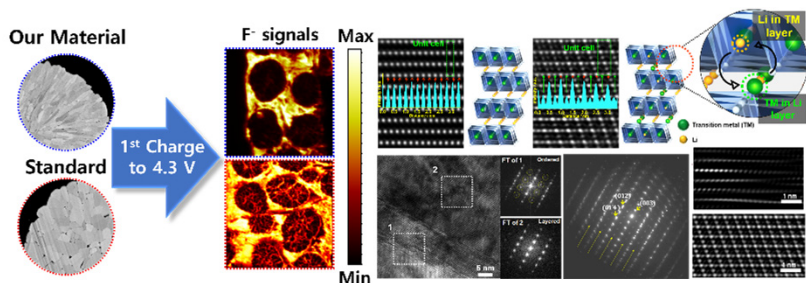
H. H. Sun, T. Pollard, O. Borodin, K. Xu, J. L. Allen, Degradation of High Nickel Li-ion Cathode Materials Induced by Exposure to Fully-Charged State and Its Mitigation, *Adv. Energy Mater.* 13, 2204360 (2023).

G.-T. Park, H. H. Sun, T.-C. Noh, F. Maglia, S.-J. Kim, P. Lamp, Y.-K. Sun, Nanostructured Co-Free Layered Oxide Cathode that Affords Fast-Charging Lithium-Ion Batteries for Electric Vehicles, *Adv. Energy Mater.* 12, 220719 (2022).

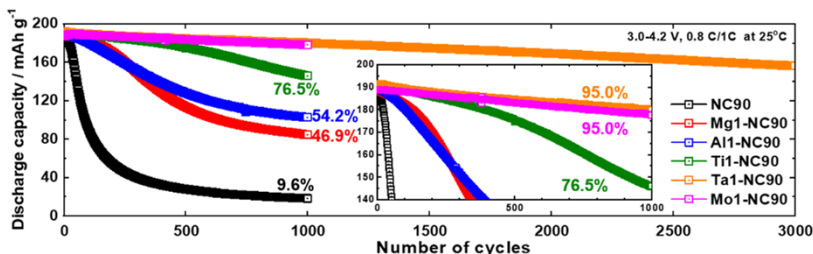
Dr. Sun's research group explores molecular phenomena and charge transport processes for the development of innovative energy materials for safer and sustainable energy storage applications.

Batteries are instrumental in supporting the energy transformation from fossil-fuel to sustainable energies, with applications ranging from portable electronics to larger grid energy storage and electric transport. This has been challenging though as batteries suffer from rising prices, cycling instabilities, and safety hazards especially at highly charged states, which in turn restrict the state-of-charge and, therefore, energy the energy density.

Our group is committed to enhancing the mechanical and chemical stabilities of next-generation energy materials to alleviating uncertainties and successful integration of batteries into our future energy systems. Specifically, the group engineers the micro- and nano-structures of material to bypass the inherent degradation pathway of battery materials to enable significantly increased cycling stabilities, even in strenuous conditions. These materials can be easily scaled-up from laboratory scale to larger pilot scale through batch type reactor synthesis to address the needs of industry. In addition, the group designs stable and conductive electrode-electrolyte interfaces through compositional engineering of electrolytes that facilitates smooth ion diffusion processes.



Micro- and nano-structure modifications



Cycling performance of engineered cathodes

Tibor Szilvási

Computational Material Design, Computational Catalysis,
Energy Storage, Interfacial Phenomena, Soft Matter



Tibor Szilvási

Assistant Professor
Ph.D. Budapest University
of Technology, 2016

Recent Publications

A. Soyemi and T. Szilvási, Calculated Physicochemical Properties of Glycerol-Derived Solvents to Drive Plastic Waste Recycling, *Industrial & Engineering Chemistry Research* 62, 6322 (2023).

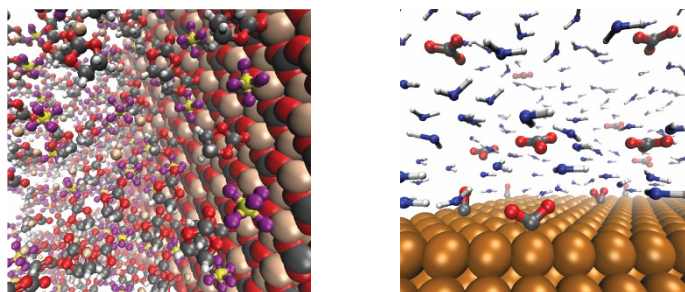
T. J. Hadlington and T. Szilvási, Accessing the main-group metal formyl scaffold through CO-activation in beryllium hydride complexes, *Nature Communications* 13, 461 (2022).

A. Soyemi and T. Szilvási, Trends in Computational Molecular Catalyst Design, *Dalton Transactions* 50, 10325 (2021)

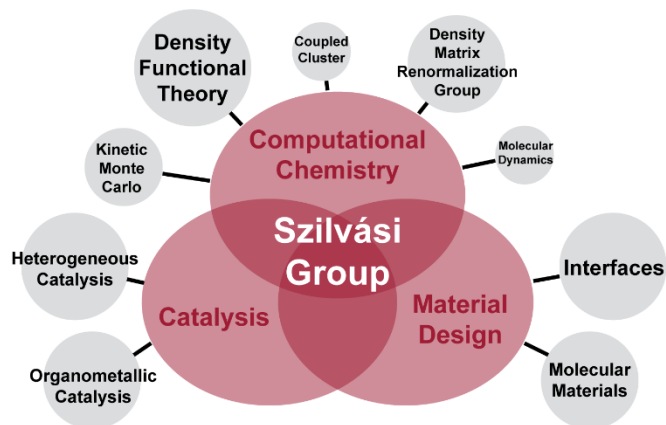
Dr. Szilvási's research group focuses on designing functional materials with well-tailored specific properties by applying computational methods.

Societal needs require the development of efficient and cheap functional materials for various technologies. Our group is committed to accelerate the development of new materials by using fast and accurate computational methods to screen potential candidates and pinpoint materials with desired properties. Using computational methods, we can potentially save millions of dollars and years of tedious experimental efforts and therefore can provide solution for pressing problems in time.

Dr. Szilvási's research group aims to focus on engineering interfaces and molecular materials. Specifically, the group intends (i) to optimize catalysts relevant for industrial processes, (ii) to identify functional materials for soft matter applications, (iii) to design complex interfaces for energy and sensor applications. To achieve these goals, Dr. Szilvási's research group also develops computational methods and protocols that can provide more accurate predictions for material design.



Representative solid-liquid interfaces



Background of Dr. Szilvási's research group

C. Heath Turner

Simulations of Nanomaterials, Computational Screening of Solvents, Environmental Catalysis Modeling, Interfacial Phenomena



C. Heath Turner

Department Head and Professor
Ph.D. Chemical Engineering
North Carolina State University,
2002

Recent Publications

G. D. Barbosa, E. Dach, X. Liu, N. Y. Yip, **C. H. Turner**, Computational and Experimental Study of Different Brines in Temperature Swing Solvent Extraction Desalination with Amine Solvents, *Desalination* 537, 115863 (2022).

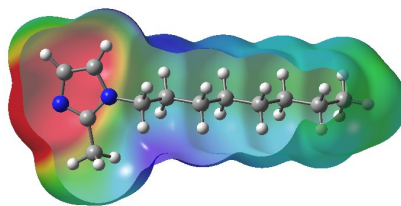
G. D. Barbosa, J. E. Bara, **C. H. Turner**, Molecular Simulation of Glycerol-Derived Triether Podands for Lithium Ion Solvation, *PCCP* 24, 9459 (2022).

X. Liu, **C. H. Turner**, Understanding Gas Absorption in Multivalent Ionic Liquids via Solute-Solvent Interaction Analyses, *Chemical Physics Letters* 786, 139204 (2022).

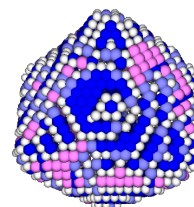
Dr. Turner's group uses computer simulations to investigate adsorption and reactions on surfaces and at interfaces. Their work helps guide the synthesis of new nanomaterials, identify new processes for environmental applications, and design new molecules for air and water purification.

The Turner group uses molecular simulations and quantum mechanical calculations to screen new materials for a variety of clean energy technologies. In the field of catalysis, we are using kinetic Monte Carlo simulations to help identify environmentally-benign routes for synthesizing large-scale commodity chemicals. Also, we are using molecular simulation tools to screen solvents for purifying wastewater and industrial gas emissions. In all projects, we work closely with experimental collaborators, in order to regularly benchmark our models and develop reliable predictions. Through this research, students acquire excellent analytical and computational skills that can be applied to many different career fields after graduation.

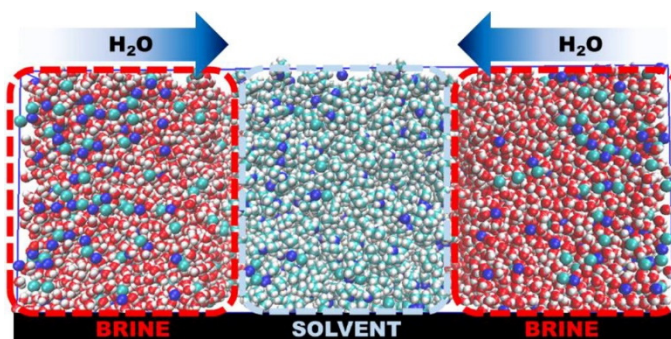
Solvents for Gas Purification



Nanoparticle Synthesis

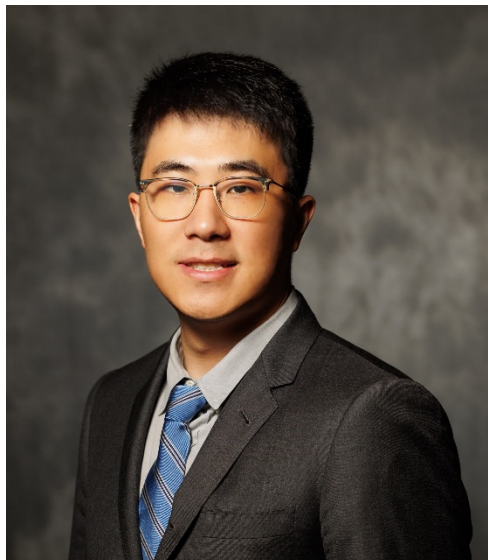


Solvent Development for Brine Treatment and Nutrient Recovery



Zhongyang Wang

Engineering Nanostructured Soft Materials for Energy and Sustainability



Zhongyang Wang

Assistant Professor
Ph.D. Energy, Environmental &
Chemical Engineering
Washington University in Saint
Louis, 2019

Recent Publications

Z. Wang, C. Wang, Y. Sun, K. Wang, J. Strzalka, S. N. Patel, P. F. Nealey, C. K. Ober, F. A. Escobedo, Ion Transport in 2D Nanostructured π -Conjugated Thieno[3,2-b]thiophene-Based Liquid Crystal, *ACS Nano*, 16, 12, 20714 (2022).

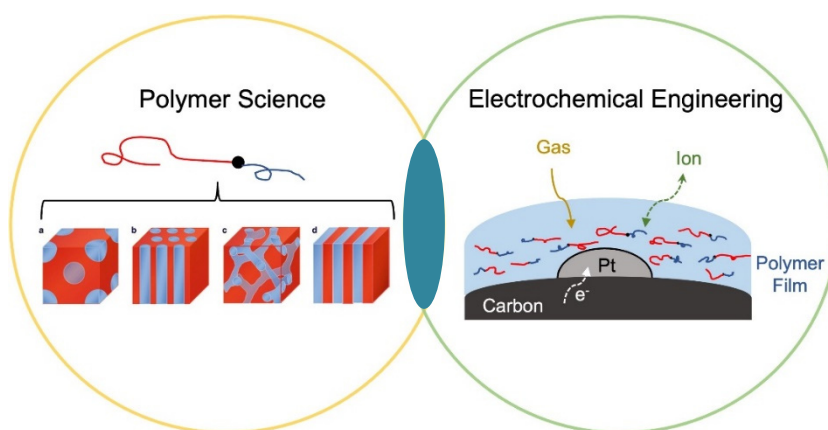
Z. Wang, J. Parrondo, C. He, S. Sankarasubramanian, V. Ramani, Efficient pH-Gradient-Enabled Microscale Bipolar Interfaces in Direct Borohydride Fuel Cells, *Nature Energy*, 4, 281 (2019).

Dr. Wang's group leverages the self-assembly of functional soft materials (block copolymers and liquid crystals) to design next-generation polymer electrolytes for energy conversion and storage.

Polymer electrolytes are at the heart of many electrochemical systems such as fuel cells, electrolyzers, and batteries. In addition, they are the key components for sustainable technologies such as electrodialysis for seawater desalination and the chloralkali process. One of the main drivers that will advance the commercialization of these sustainable processes is the development of mechanical robust, highly ion conductive, ion selective, and chemically resistive polymer electrolytes.

The Wang group aims to empower high-performance electrochemical systems and sustainable technologies by solving fundamental problems at the interface of polymer science and electrochemical engineering. The group focuses on three distinct areas: (1) understanding ion/electron transport in nanostructured block copolymers and liquid crystals, (2) developing efficient pH-gradient-enabled microscale bipolar interfaces for water and CO₂ electrolysis, and (3) engineering sub-2 nm structured liquid crystals for efficient water treatment and energy storage.

Overall research interest



Steven Weinman

Membranes for Water Purification, Surface Science,
Solvent Desalination, Water and Wastewater Treatment



Steven T. Weinman
Assistant Professor
Ph.D. Chemical Engineering
Clemson University, 2018

Recent Publications

S. Habib, B. E. Larson, **S. T. Weinman**, Effect of Surfactant Structure on MPD Diffusion for Interfacial Polymerization, *Journal of Membrane Science Letters* 3,100055 (2023).

S. Qian, L. M. Ward, L. S. Rakers, **S. T. Weinman**, and J. E. Bara, 1-Propyl-4(5)-Methylimidazole isomers for Temperature Swing Solvent Extraction, *Molecules* 27, 5583 (2022).

S. Habib and **S. T. Weinman**, Modification of polyamide reverse osmosis membranes for the separation of urea, *Journal of Membrane Science* 655, 120584 (2022)

Dr. Weinman's group focuses on functionalizing and synthesizing membranes and new solvents to improve current water treatment technologies.

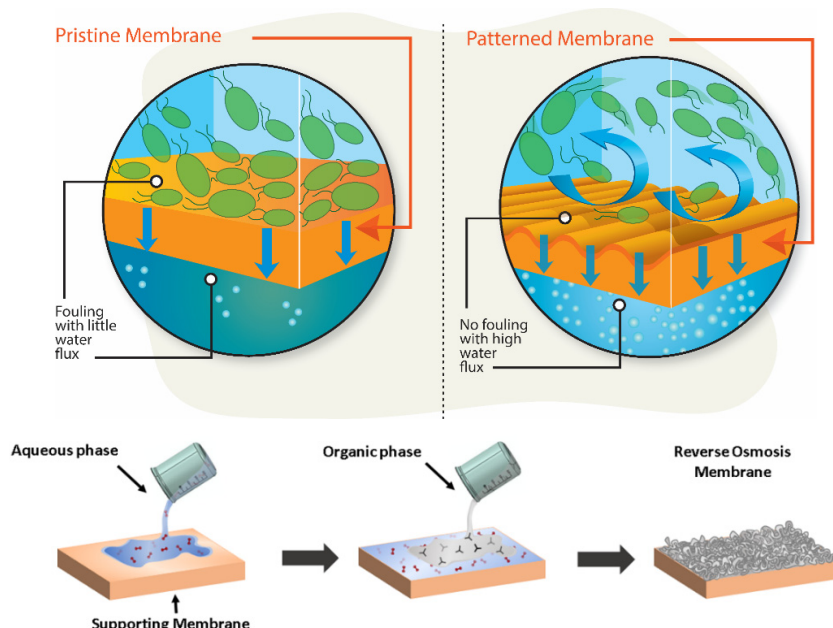
Membranes are semi-permeable barriers that separate substances when a driving force is applied across the membrane. The Weinman group works to provide solutions to current environmental challenges by developing new membrane and solvent technologies.

The Weinman Group focuses on synthesizing and studying the fundamental properties of thin-film composite membranes for nanofiltration and reverse osmosis applications. This will allow us to better understand what factor(s) influence membrane properties and utilize this understanding to enable new separations.

Progressive decline in water permeability due to fouling is one of the largest costs associated with membrane processes in water treatment. My research focuses on surface modifying membranes to reduce various types of fouling (oil, biological, scaling, etc.).

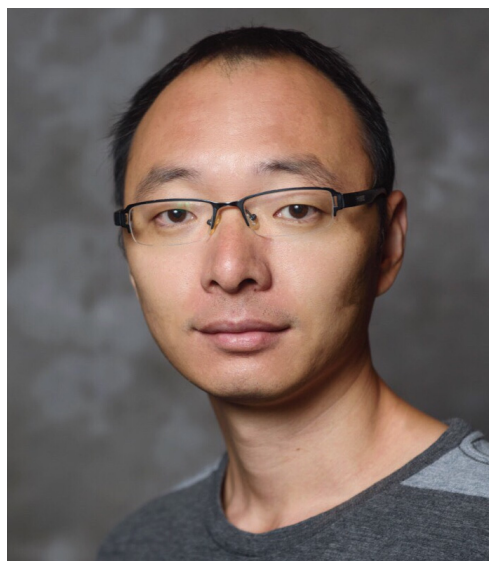
Another area of interest is creating membrane adsorbers and solvents to capture compounds of interest. There is a need to selectively remove persistent pollutants and high value products from numerous water sources.

Lastly, the Weinman Group is exploring new solvents for brine desalination where membranes cannot be used.



Chao Zhao

Polymers, Biomaterials, Drug Delivery, Tissue Engineering



Chao Zhao

Assistant Professor
Ph.D. Chemical Engineering
The University of Akron, 2013.

Recent Publications

C. Zhao, A. Liu, C. Santamaria, A. Shomorony, T. Ji, T. Wei, R. Yang, D. Kohane, Polymer-tetrodotoxin conjugates to prolonged duration local anesthesia with minimal toxicity, *Nature Communications*, 10 (1), 2566 (2019).

C. Zhao, S. Tian, Q. H. Liu, K. M. Xiu, L.L. Lei, Z. Wang, P. X. Ma, Biodegradable nanofibrous temperature-responsive gelling microspheres for heart regeneration, *Advanced Functional Materials*, 00776. (2020).

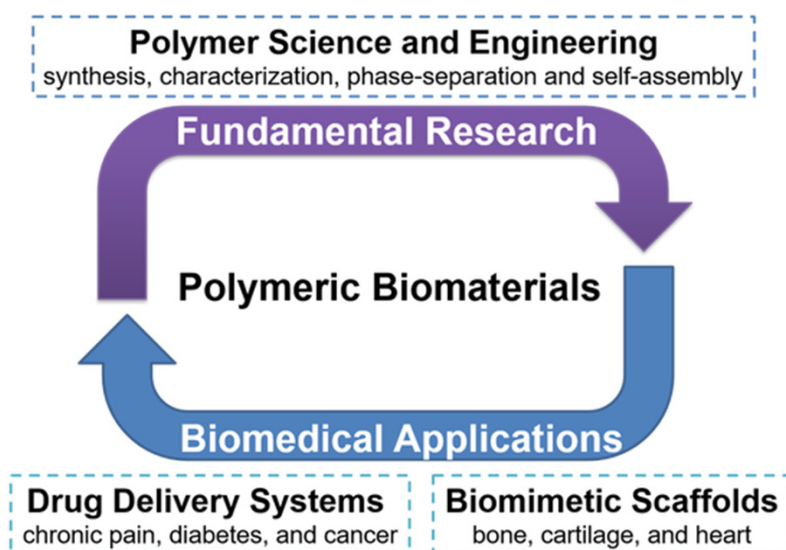
X. Li, Y. Zhao, C. Zhao, Applications of capillary action in drug delivery, *iScience*, 24(7):102810 (2021).

The Zhao Lab develops novel polymeric biomaterials for various biomedical applications, with emphasis on drug delivery and tissue engineering. The projects are driven by developing new technologies for the treatment of specific diseases.

Tetrodotoxin (TTX) is a potent neurotoxin that blocks voltage-gated sodium channels on the cell surface. TTX is 3000 times more potent analgesic than morphine without the opioid-like side effects. However, the principal reason that TTX has not achieved clinical use despite their great potency is concern over their associated systemic toxicity. TTX toxicity causes neural blockade and muscular weakness resulting in diaphragmatic paralysis leading to respiratory arrest and death. The severe systemic toxicity limits the dosing of TTX, and therefore limits the maximal duration of analgesic effects achievable.

The primary objective of Zhao's research is to use materials-based approaches to address the limitations imposed by the toxicity of TTX, and to move toward clinical translation of TTX for the pain treatment.

Other projects in Zhao lab include the development of polymeric vectors for gene therapy, and biomimetic scaffolds to enhance delivery of stem cells for tissue regeneration.



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