THE UNIVERSITY OF

ALABAMA®

Graduate Research Opportunities

2021/2022

THE UNIVERSITY OF ALABAMA® | College of Engineering

Chemical and Biological Engineering

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 – SZILVÁSI – TURNER

Computational/Thermodynamics

BARA – ESFAHANI – SHEEHAN – SZILVÁSI – TURNER

Electronic Materials and Devices

GUPTA – HUANG – KLEIN – KOH – PENG – WUJCIK

Energy/Environmental/Water

BARA – ESFAHANI – KOH – RITCHIE – SHEEHAN – WEINMAN – WUJCIK

Membranes and Polymers

BARA – BRAZEL – ESFAHANI – KOH – RITCHIE

WEINMAN – WUJCIK – ZHAO

FACULTY

Yuping Bao, Ph.D., Washington

Jason E. Bara, Ph.D., Colorado

Christopher S. Brazel, Ph.D., Purdue

Milad Esfahani, Ph.D., Tenn Tech

Arunava Gupta, Ph.D., Stanford

James W. Harris, Ph.D. Purdue

Qiang Huang, Ph.D., LSU

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

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

Amanda Koh, Ph.D., Rensselaer

Russell Mumper, Ph.D., Kentucky

Qing Peng, Ph.D., NC State

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

Stephen Ritchie, Ph.D., Kentucky

James Sheehan, Ph.D., Penn State

Ryan Summers, Ph.D., Iowa

Tibor Szilvási, Ph.D., BME, Hungary

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

Steven Weinman, Ph.D., Clemson

John M. Wiest, Ph.D., Wisconsin

Evan K. Wujcik, Ph.D., Akron

Chao Zhao, Ph.D., Akron

Graduate Coordinator

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

THE UNIVERSITY OF ALABAMA® | College of Engineering

Chemical and Biological Engineering

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, Prof. Brazel; Humboldt Research Prize, Prof. Gupta)!***

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/

THE UNIVERSITY OF ALABAMA® | College of Engineering

Chemical and Biological Engineering

Research Support

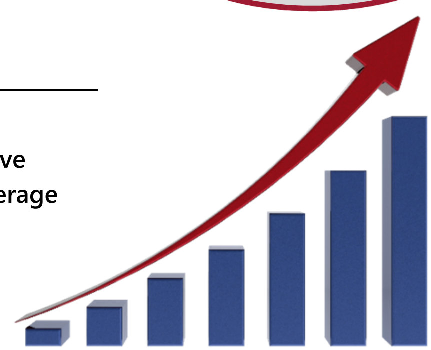
Funding the Best and Brightest Ideas

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 100% 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 100% per year!



Research Funding

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.

THE UNIVERSITY OF ALABAMA® | College of Engineering
Chemical and Biological Engineering

Faculty Research Profiles

2021/2022

Yuping Bao

Nano-Bio Interface Laboratory - Multifunctional Nanostructures for Simultaneous Imaging and Therapy, and Drug Discovery

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

Recent Publications

J. Horne, S. Mansur, and **Y. Bao**, Sodium Ion Channels as Potential Therapeutic Targets for Cancer Metastasis, *Drug Discovery Today*, in press (**2020**).

J. Sherwood, J. Sowell, N. Beyer, J. Irvin, C. Stephen, A. Antone, **Y. Bao**, M. L. Ciesla, Cell-Membrane Coated Iron Oxide Nanoparticles for Isolation and Specific Identification of Drug Leads from Complex Matrices, *Nanoscale* 11, 6352 (**2019**).

J. Sherwood, M. Rich, K. Lovas, J. Warram, M. S. Bolding, **Y. Bao**, T_1 Enhanced MRI-visible Nanoclusters for Imaging-Guided Drug Delivery, *Nanoscale* 9, 11785 (**2017**).

Dr. Bao's group focuses on designing novel multifunctional nanoparticles for biomedical applications, such as targeted drug delivery, bio-imaging, and drug discovery.

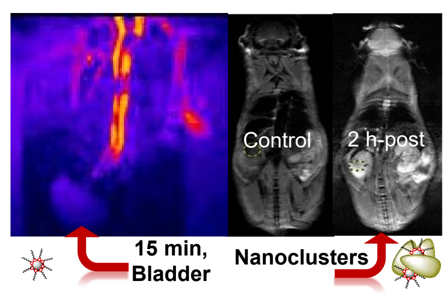
Magnetic nanoparticles have significantly advanced cancer treatments through targeted drug delivery and localized therapy. Magnetic nanoparticles further make simultaneous therapy and diagnosis possible as magnetic resonant imaging (MRI) contrast agents.

One of the unique aspects of Bao's research is the creation of a suite of iron oxide nanoparticles of different shapes as MRI contrast agents and for other biotechnology related applications. These shapes include spheres, cubes, nanowires, plates, flowers, etc.

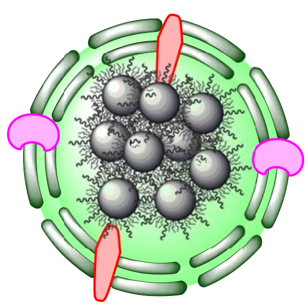
Much of Dr. Bao's work is directly related to the engineering of material interfaces. Her group developed a facile method to attach various molecules onto nanoparticle surfaces for water solubility and desirable functionality, such as tumor targeting.

In collaboration with UAB and Biological Science Department at UA, Bao's group also designs nanostructures for the delivery of modulator drugs to the brain and nanostructures for drug screening from complex matrices.

T_1 enhanced MRI-visible nanoclusters with increased blood circulation time



Cell-membrane coated magnetic nanoparticles for drug screening



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Jason E. Bara

Advanced Polymers and Composites, Gas Separation Membranes "Green" Chemistry, Ionic Liquids, 3-D Printing, Polymer Upcycling and Depolymerization, Big Data, Chemical Engineering Mobile Apps

Jason E. Bara

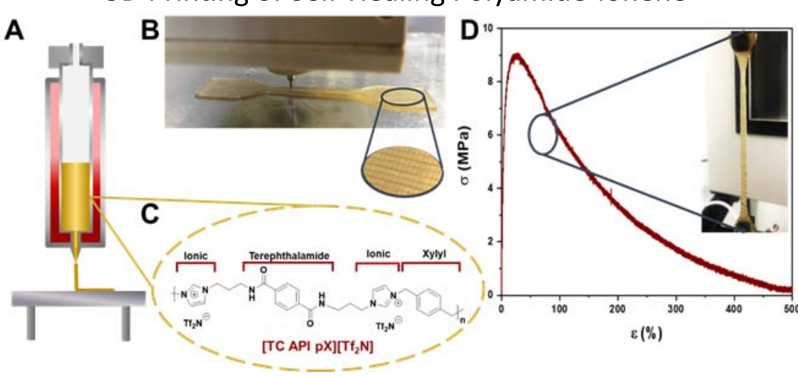
Professor
Ph.D. Chemical Engineering
University of Colorado at Boulder, 2007

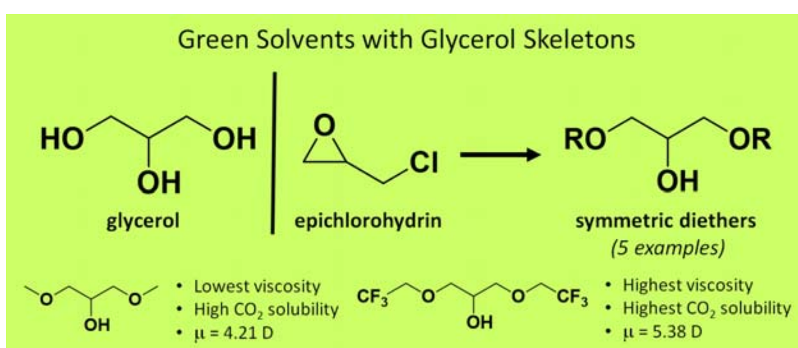
Dr. Bara's research group is focused on development of advanced polymer materials, energy efficient separations, green chemical manufacture, 3-D printing, big data, and scientific apps for iPhones and iPads.

Dr. Bara is a recognized leader in the design and synthesis of advanced polymers and composites based on ionic liquids. These materials provide unprecedented opportunities to create stable nanostructured materials with highly tunable chemical and physical properties for applications including gas separation membranes, water purification, superabsorbents, shape-memory and self-healing, and 3-D printing.

Dr. Bara's group is also very active in the synthesis and study of new "green" solvents and their roles in polymer upcycling and depolymerization. Dr. Bara has also developed several widely used apps for iPhones/iPads including Chemical Engineering AppSuite.

3D Printing of Self-Healing Polyamide-Ionene





Recent Publications

K. E. O'Harra, N. Sadaba, M. Irigoyen, F. Ruipérez, R. Aguirresarobe, H. Sardon, and **J. E. Bara**, Nearly Perfect 3D Structures Obtained by Assembly of Printed Parts of Polyamide Ionene Self-Healing Elastomer, *ACS Appl. Polym. Mater.* (**2020**). doi:10.1021/acsapm.0c00799

S. Qian, X. Liu, G. P. Dennis, C. H. Turner, and **J. E. Bara**, Properties of Symmetric 1,3-Diethers Based on Glycerol Skeletons for CO_2 Absorption, *Fluid Phase Equilibr.* 521, 112718 (**2020**).

jbara@eng.ua.edu ◦ http://jbara.eng.ua.edu/ ◦ (205) 348-6836 ◦ Twitter: @ProfBara

Christopher Brazel

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

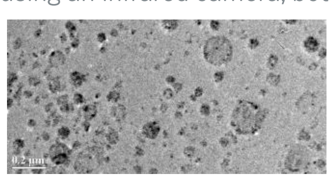
Christopher Brazel
Associate Professor
Ph.D. Chemical Engineering
Purdue University, 1997

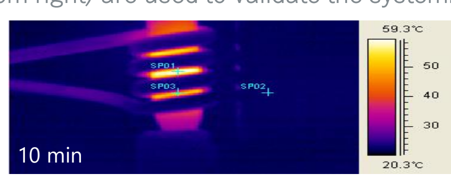
The Brazel Laboratory is interested in developing and understanding the chemical and biological properties of materials for medical, biopharmaceutical, and chemical processing applications. Recent foci in the lab include: (1) developing a robust toxicology assay to evaluate polymer films for single-use 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.





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**).

cbrazel@eng.ua.edu ◦ cbrazel.people.ua.edu ◦ (205) 348-9738

Milad Rabbani Esfahani

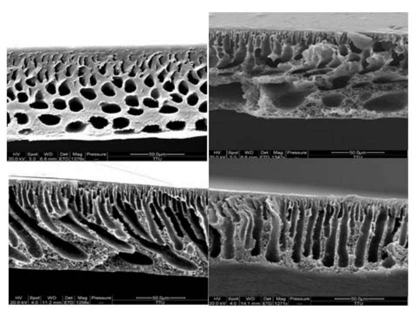
Functionalized Membranes For Sustainable Water and Energy Production, Water Purification and Desalination, Nanomaterials Environmental Safety

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

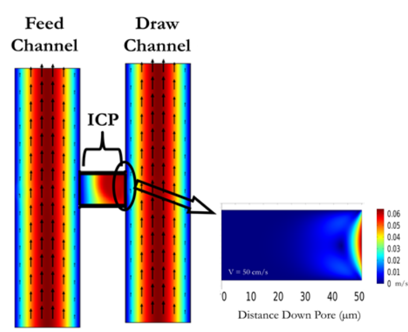
Dr. Esfahani 's group uses a multidisciplinary approach to develop novel functionalized membranes with ultimate goal of water -wastewater treatment and energy production.

Our research field is at the interface of several disciplines including separation science, nanotechnology, materials science and colloid science that links to the water-energy-food nexus. In the field of functionalized membranes, we are developing catalytic membranes with self-cleaning properties where they can provide higher permeability and less fouling. . Our research group will develop different strategies to incorporate nanoparticles with specific properties such as photo catalytic activity of titanium dioxide nanoparticles, highly adsorptive properties of multiwall carbon nanotube, anti-bacterial properties of silver nanoparticles, and high absorptive properties of gold nanoparticles to the polymeric structure of the membranes for creation of advanced self-cleaning membranes. We use both computational and experimental approaches to design engineered membranes for water desalination, water purification and energy production. Also, in the field of nanomaterials environmental safety, we are studying the transport and fate of nanomaterials in aquatic environment.

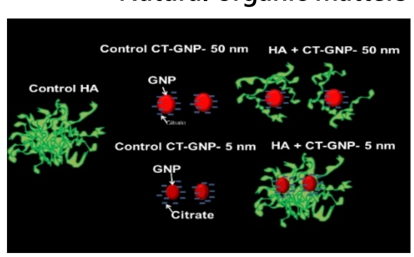
Nano-composite Membranes Fabrication and Characterization

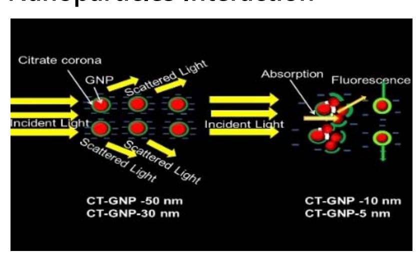


CFD Modeling of Transport Phenomena in Membranes



Natural organic matters – Nanoparticles Interaction





Recent Publications

M. R. Esfahani, V. L. Pallema, H. A. Stretz, M. J. M. Wells, Core-Size Regulated Aggregation - Disaggregation of Citrate-Coated Gold Nanoparticles (5–50 nm) and Dissolved Organic Matter: Extinction, Emission, and Scattering Evidence, *Spectro. Acta Part A: Molecular and Biom. Spectroscopy* 189, 415 (**2018**).

M. R. Esfahani, E. M. Languri, M. R. Nunna, Effect of Particle Size and Viscosity on Thermal Conductivity Enhancement of Graphene Oxide Nanofluid, *Inter. Communications in Heat and Mass Transfer 76, 308* (**2016**).

mesfahani@eng.ua.edu ◦ http://mesfahani.people.ua.edu ◦ (205) 348-8836

Arunava Gupta

Controlled Synthesis and Assembly of Nanomaterials and Nanostructures

Arunava Gupta
Professor
Ph.D. Chemical Physics
Stanford University, 1980

Recent Publications

K. Ramasamy, R. K. Gupta, S. Palchoudhury, S. Ivanov, and **A. Gupta**, Layer-Structured Copper Antimony Chalcogenides ($CuSbSe_xS_{2-x}$): Stable Electrode Materials for Supercapacitors, *Chem. Mater.* 27, 379 **(2015).**

Z. Zhou, G. J. Bedwell, R. Li, N. Bao, P. E. Prevelige, and **A. Gupta**, P22 Virus-like Particles Constructed Au/CdS Plasmonic Photocatalytic Nanostructures for Enhanced Photoactivity, *Chem. Commun.* 51, 1062 **(2015).**

Z. Shan, D. Clayton, S. Pan, P. S. Archana, and **A. Gupta**, Visible Light Driven Photoelectrochemical Properties of Ti@TiO_2 Nanowire Electrodes Sensitized with Core-Shell Ag@Ag_2S Nanoparticles, *J. Phys. Chem. B* 118, 14037 **(2014).**

Dr. Gupta's group focuses on controlled synthesis and assembly of nanomaterials and nanostructures, with emphasis on the exploration and manipulation of materials' physical and chemical properties and their potential applications.

Spintronics, also known as magneto-electronics, is an emerging technology which exploits the intrinsic spin of electrons and its associated magnetic moment, in addition to its fundamental electronic charge, in solid-state devices. Spintronics exploits electron spin, creating a new class of devices that can potentially be scaled down to nano-dimensions and can also provide additional functionality. The group is interested in the growth and characterization of novel magnetic thin films by a variety of deposition techniques, including chemical vapor deposition, pulsed laser deposition, etc. for the fabrication of devices, such as magnetic tunnel junctions and spin-based semiconductors, and their application for storage, memory, and logic-based devices.

Nanomaterials are of great interest for a wide range of applications, including catalysis, data storage, biotechnology/biomedicine, etc. In particular, the synthesis of monodisperse uniform-sized nanocrystals using solution-based methods is of key importance for these applications because of their strong dimension-dependent physical and chemical properties. Dr. Gupta's research group is interested in the synthesis of functional oxides and chalcogenides in the form of nanoparticles and other nanostructures with controlled shape, size, structure, etc.

In addition to traditional methods for the synthesis of inorganic nanomaterials, novel approaches are being developed that exploit advances in biotechnology. The bio-inspired approach to materials synthesis has successfully utilized cells, viruses, and biomolecules, such as nucleic acids, proteins, etc., to produce inorganic nanomaterials with controlled crystal morphology, phase structure, and size, under mild conditions.

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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**).

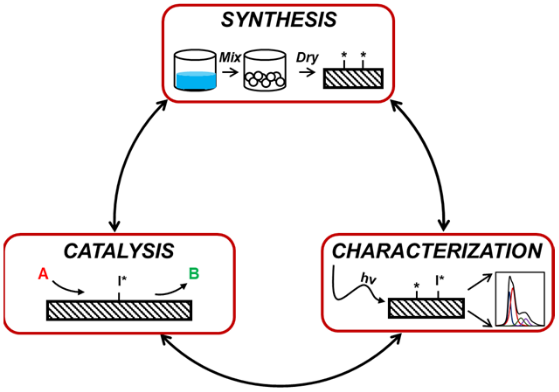
J. W. Harris, A. V. Verma, J. A. Arvay, A. J. Shih, W. N. Delgass, and F. H. Ribeiro, Consequences of Product Inhibition in the Quantification of Kinetic Parameters, *J. Catal.* 389, 468 (**2020**).

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.

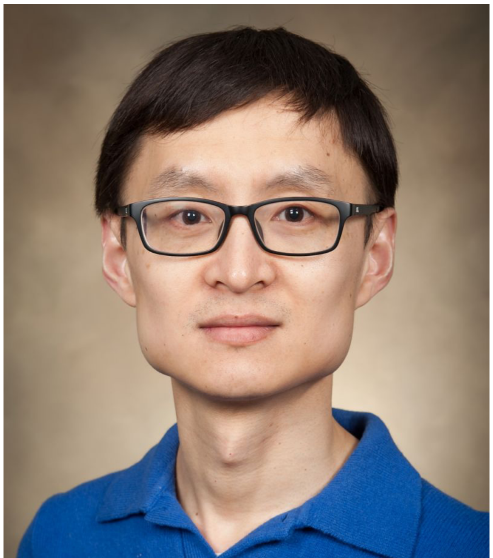


A second area of research involves upgrading of oxygenates derived from biomass. These highly-functionalized molecules can act as platform molecules for production of fuels, polymer precursors, solvents, flavorings, perfumes, and pharmaceutical precursors. Production of these high-value chemicals currently 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.

james.harris@eng.ua.edu ◦ http://che.eng.ua.edu/people/james-harris/ ◦ (205) 348-0813
Twitter: @JWHarrisCatal

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 Electro-deposition 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**).

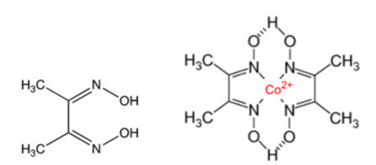
S. De, J. White, T. Brusuelas, C. Patton, A. Koh, and **Q. Huang**, Electrochemical Behavior of Protons and Cupric Ions in Water in Salt Electrolytes with Alkaline Metal Chloride, *Electrochim. Acta.* 228, 135852 (**2020**).

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

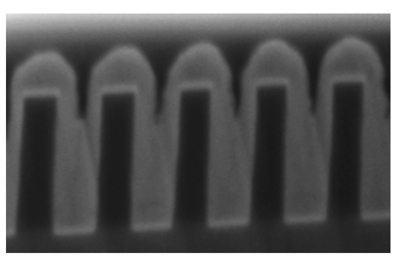
Electrochemical reactions are chemical reactions that involve electron transfer. Dr. Huang's current research focuses on such reactions in conjunction with materials sciences, investigating the impacts of the chemistry and process on the material structure and properties. Two example applications are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

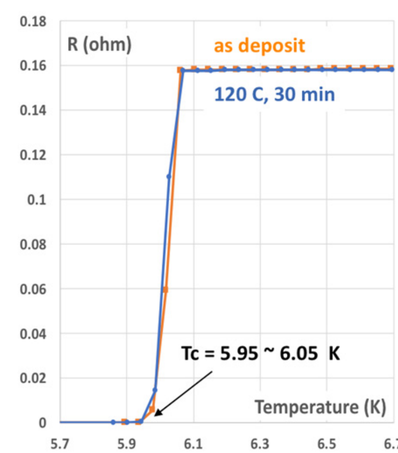
The convenience of our daily life and the development of modern technology heavily rely on the advancement of microelectronic and semiconductor devices. Interconnect is a nanometer sized network of metal wires in integrated circuits, enabling the communication between each semiconductor devices (transistors). 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)



$Co^{2+} + 2e \rightarrow Co$ $[CoL_2]^{2+} + 2e \rightarrow Co + 2L$





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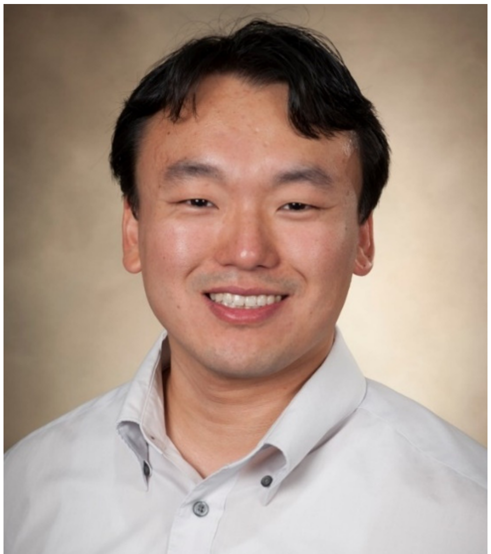
Yonghyun (John) Kim

Bioengineering, Oncology, Systems Biology, Translational Medicine



Yonghyun (John) Kim

Associate Professor
Ph.D. Chemical Engineering
Univ. Maryland Baltimore County, 2008

Recent Publications

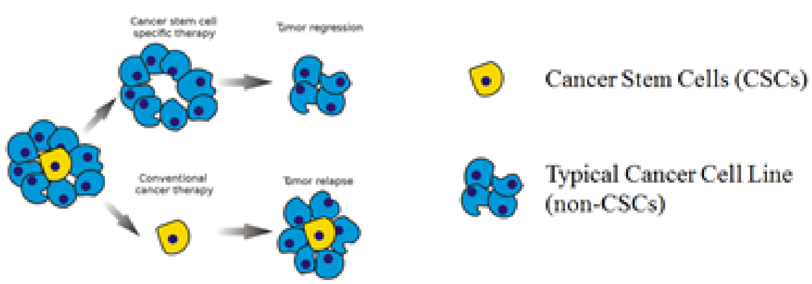
S. R. Brown, J. C. Bates, A. D. Avera, **Y. Kim**, Relationship between Stemness, Reactive Oxygen Species, and Epithelial-to-Mesenchymal Transition in Model Circulating Tumor Cells. *Cells Tissues Organs*. Jun:1-12 (**2021**).

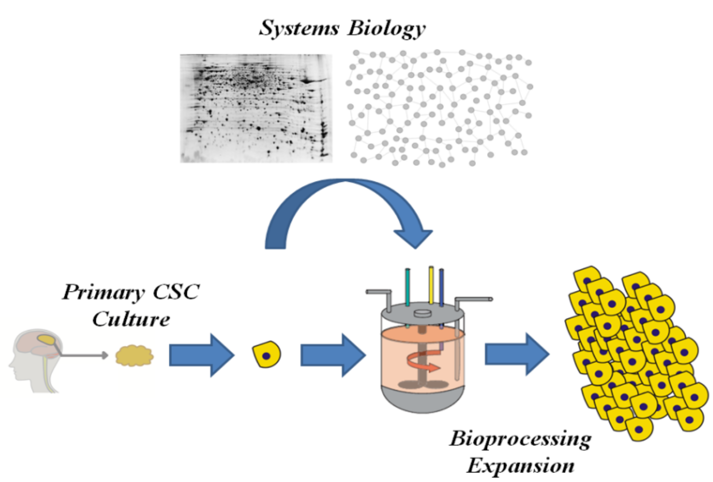
H.-A. Park, S. R. Brown, **Y. Kim**, Cellular Mechanisms of Circulating Tumor Cells During Breast Cancer Metastasis, *Int. J. Mol. Sci.* 21(14):5040 (**2020**).

J. W. Magrath, W. R. Raney, **Y. Kim,** In vitro Demonstration of Salinomycin as a Novel Chemotherapeutic Agent for the Treatment of SOX2-positive Glioblastoma Cancer Stem Cells. *Oncol Rep*. 44:777-785 (**2020**).

The Kim laboratory is working on bioprocessing expansion of cancer stem cells to better assist translational medicine. Cancer stem cells (CSCs) are considered the stem cell-like pluripotent cancer cells that cause relapse in patients even after the most rigorous treatment.

Pharmaceutical companies, however, typically use several decades-old cancer cell lines during their drug development because, among many reasons, (1) CSCs are hard 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 large scale quantities of CSCs using engineering principles and systems biology tools (e.g. proteomics) for the mass production of CSCs from primary patient tissues and cell culture. By doing so, they hope to assist in the drug development by providing a more relevant and closer-to-clinic resource of cancer cells.





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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

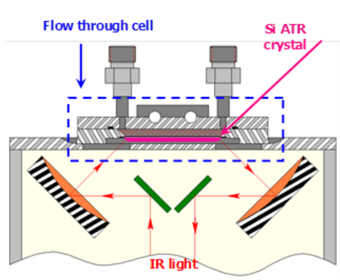
K. J. Li, L. Zhang, D. A. Dixon, **T. M. Klein**, Undulating Topography of HfO_2 Thin Films Deposited in a Mesoscale Reactor Using Hafnium (IV) tert Butoxide, *AICHE J.* 57, 2989 (**2011**).

N. Li, M. Liu, Z. Zhou, N. X. Sun, D. V. B. Murthy, G. Srinivasan, **T. M. Klein**, et al., Electrostatic Tuning of Ferromagnetic Resonance and Magnetoelectric Interactions in Ferrite-piezoelectric Heterostructures Grown by Chemical Vapor Deposition, *Appl. Phys. Lett.* 99, 192502 (**2011**).

As electronic, magnetic and photonic devices become more sophisticated, there is an ever-pressing need to fully understand the physics and chemistry of solid interfaces. Technologies such as spin valves, field effect transistors, and nano-laminate optical coatings are all 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.

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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

Koh, A., Sietins, J., Mrozek, R., Slipher, G., Deformable liquid metal polymer composites with independently tunable electronic and mechanical properties, *J. Mater. Res.* 33, 2443 (**2018**).

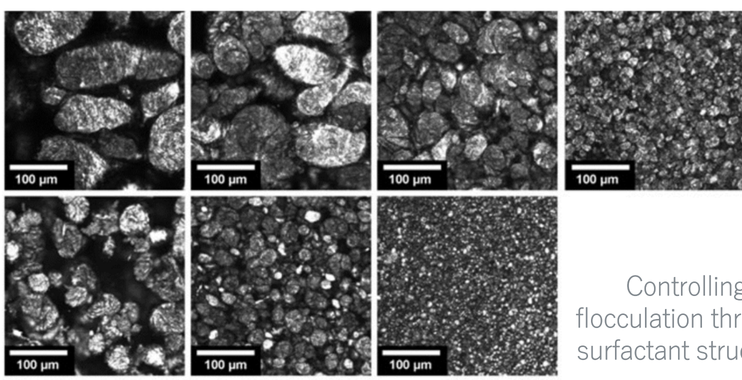
Koh, A., Mrozek, R., Slipher, G., Characterization and Manipulation of Interfacial Activity for Aqueous Galinstan Dispersions, *Adv. Mater. Interfaces* 5, 1701240 (**2018**).

Koh, A., Hwang, W., Zavalij, P. Y., Chun, S., Slipher, G., and Mrozek, R., Solidification and melting phase change behavior of eutectic gallium-indium-tin. *Materialia* 8, 100512 (**2019**).

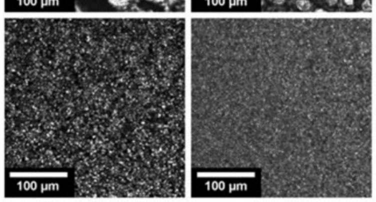
Dr. Koh's group focuses on engineering multifunctional materials through the intentional design of interfaces. Current research focuses on materials for soft robotics, stretchable electronics, sensing, and environmental remediation.

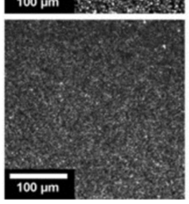
As devices become more advanced in the fields of defense, health, and manufacturing, it is no longer enough for materials to have a single function or a be useful to only a single application. Materials that are responsive and multifunctional are key to creating robust, practical, and adaptive systems. 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 sensing (ex. heavy metals and petroleum derivatives).

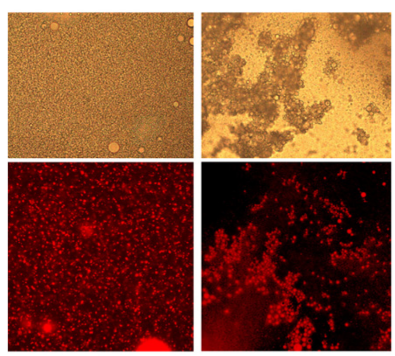


Controlling flocculation through surfactant structure





Liquid metal in PDMS dielectric dispersions



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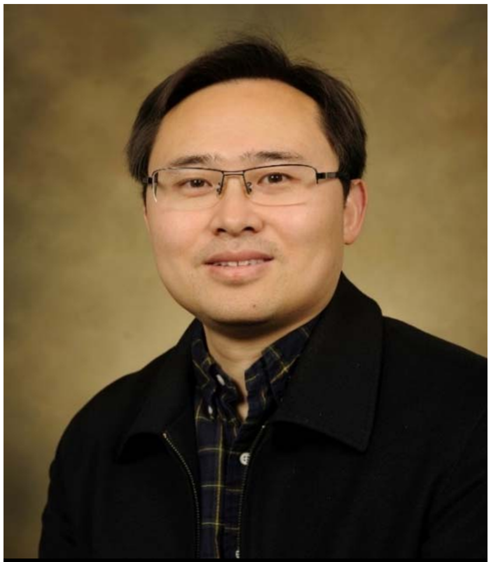
Qing Peng

Surface/Interfacial Engineering Group



Qing Peng
Assistant Professor
Ph.D. Chemical Engineering
North Carolina State University, 2009

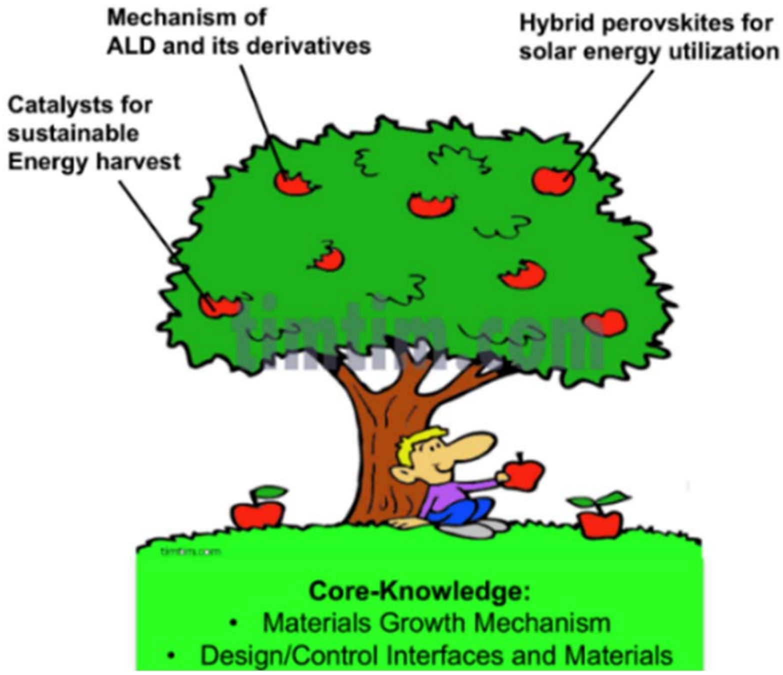
Recent Publications

H. Yan, Z. Liu, S. Yang, X. Yu, T. Liu, Q. Guo, J. Li, R. Wang, and **Q. Peng**, Stable and Catalytically Active Shape-Engineered Cerium Oxide Nanorods by Controlled Doping of Aluminum Cations, *ACS Applied Materials & Interfaces* 12, 37774 (**2020**).

X. Yu, H. Yan, and **Q. Peng**, Improve the Stability of Hybrid Halide Perovskite via Atomic Layer Deposition on Activated Phenyl-C61 Butyric Acid Methyl Ester, *ACS Applied Materials & Interfaces* 10, 28948 (**2019**).

Dr. Peng's group focuses on understanding and applying vapor-substrate reactions to synthesize novel materials and to control the material interfaces (down to the atomic level) in order to improve the performance of materials and devices in microelectronics, solar energy conversion, separations.

We investigate the nucleation and growth materials by in-situ/ex-situ analytic methods in order to understand surface/interfacial chemistry and micro-structures of materials, and establishing the structure-property relationship of materials. Dr. Peng works on the following projects:



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Shreyas Rao

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

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

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.

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**).

Stephen Ritchie

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

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

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.

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**).

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James D. Sheehan

Chemical Reactions in Supercritical Fluids, *in situ* Spectroscopy for Evaluating Reaction and Phase Behavior, Chemical Kinetic Modeling

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

Dr. Sheehan's group uses experimental and modeling approaches for evaluating reaction kinetics and phase behavior of mixtures in supercritical fluids. Their research develops sustainable processes for synthesizing commodity and fine chemicals.

Supercritical fluids (SCFs) are compressible fluids consisting of chemical species under temperatures and pressures exceeding their critical point. The properties of SCFs (e.g., density, viscosity, diffusivity, etc.) are intermediate of those of gases and liquids, and their compressibility facilitates "tuning" of their properties by adjusting temperature and/or pressure. As such, the tunable properties of SCFs allows for enhanced control over phase behavior and solubility of chemical species in SCFs, which in turn, has implications for the design of reaction and separation processes.

The Sheehan group investigates the phase behavior and solubility of chemical species in SCFs and evaluates the chemical kinetics of associated reactions of interest. They evaluate SCF systems via *in situ* spectroscopic and *ex situ* analytical methods and leverage computational modeling tools for quantifying chemical kinetics and optimizing process conditions. The overarching research objective of the Sheehan group is to develop novel and sustainable chemical processes that mitigate the use of toxic chemicals and promote process intensification by integrating reaction and separation unit operations.

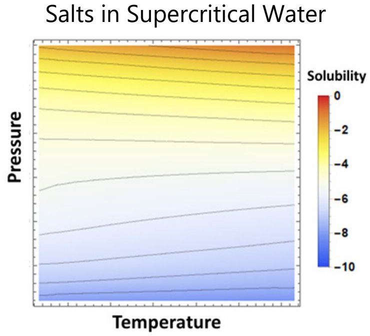
Recent Publications

J. D. Sheehan and P.E. Savage, Reaction Pathways and Kinetics of Tryptophan in Hot , Compressed Water. *Chem. Eng. J.* 390, 124600 (**2020**).

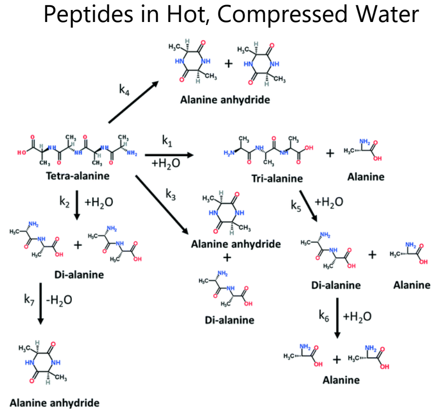
J.D. Sheehan, A. Abraham, and P.E. Savage, Reaction Pathways and Kinetics for Tetra-Alanine in Hot, Compressed Liquid Water. React. Chem. Eng. 4, 1237–1252 (**2019**).

Research Examples

Phase Behavior
Solubility of Potassium Phosphate Salts in Supercritical Water



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



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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.

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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

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

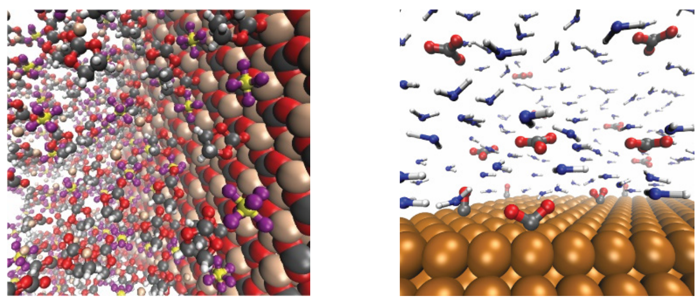
Zsolt Benedek, Marcell Papp, Julianna Oláh, and **Tibor Szilvási**, Demonstrating the Direct Relationship between Hydrogen Evolution Reaction and Catalyst Deactivation in Synthetic Fe Nitrogenases, *ACS Catalysis* 10, 12555 (**2020**).

Y. Wang, **T. Szilvási**, S. Yao, and M. Driess, A Bis(silylene)-Stabilized Diphosphorus Compound and Its Reactivity as a Monophosphorus Anion Transfer Reagent, *Nature Chemistry* 12, 801 (**2020**).

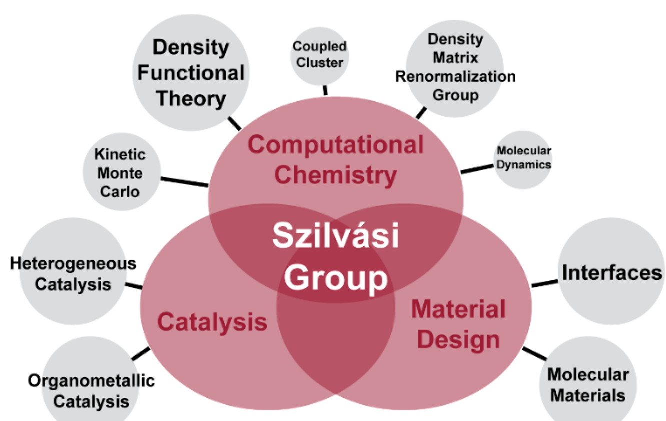
Dr. Szilvási's research group focuses on designing functional materials with well-tailored specific properties by applying computational methods.

Societal needs require to develop 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

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C. Heath Turner

Simulations of Nanomaterials, Computational Screening of CO_2 Solvents, Environmental Catalysis Modeling, Interfacial Phenomena

C. Heath Turner
Professor
Ph.D. Chemical Engineering
North Carolina State University, 2002

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 catalysts for environmental applications, and design unique solvent molecules for CO_2 separation technologies.

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 an environmentally-benign route for synthesizing propylene oxide using gold-based nanoparticles. Also, we are using molecular simulation tools to screen solvents for producing thermoelectric materials (such as Bi_2Te_3), which can be used to capture waste heat from a variety of sources. In terms of CO_2 capture, we are developing efficient simulation tools for quickly screening and identifying effective solvents and polymers for CO_2 capture applications. In all projects, we work closely with experimental collaborators, in order to regularly benchmark our models and develop reliable predictions.

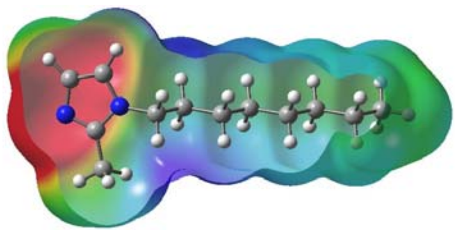
Recent Publications

P. Sappidi, J. E. Bara, and **C. H. Turner,** Molecular-Level Behavior of Imidazolium-Based Ionic Liquid Mixtures, *Chem. Eng. Sci.* 229, 116073 (**2021**).

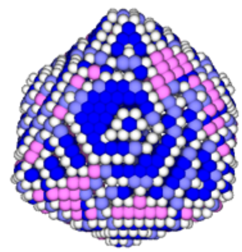
H. Atkinson, J. E. Bara, and **C. H. Turner,** Molecular-Level Analysis of the Wetting Behavior of Imidazolium-Based Ionic Liquids on Bismuth Telluride Surfaces, *Chem. Eng. Sci.* 211, 115270 (**2020**).

X. Liu, K. E. O'Harra, J. E. Bara, and **C. H. Turner**, Molecular Insight into the Anion Effect and Free Volume Effect of CO_2 Solubility in Multivalent Ionic Liquids, *PCCP* 22, 20618 (**2020**).

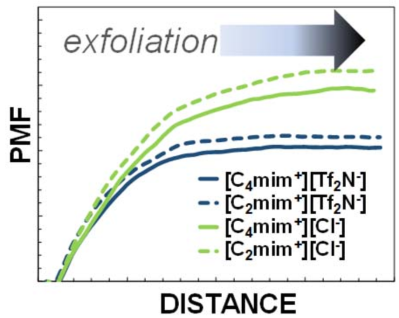
Solvents for CO_2 Absorption

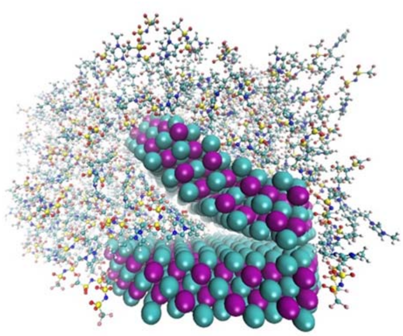


Nanoparticle Synthesis



Exfoliation of Nanomaterials for Energy Harvesting





Steven Weinman

Membranes for Water Purification, Membrane Fouling, Surface Science, Water and Wastewater Treatment

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

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

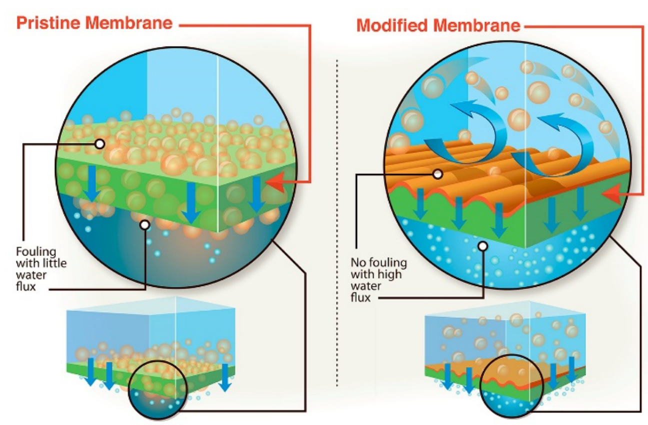
Membranes are semi-permeable barriers that separate substances when a driving force is applied across the membrane. The Weinman group works to provide solutions to current environmental and wastewater challenges by developing new membrane technologies.

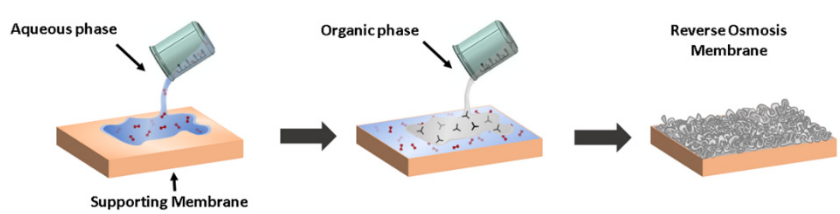
The Weinman Group focuses on synthesizing and studying the fundamental properties of thin-film composite membranes for nanofiltration and reverse osmosis applications. This will allow us to better understand what factor(s) influence membrane properties and utilize this understanding to enable new separations.

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 project area involves creating membrane adsorbers and solvents to capture compounds of interest. There is a need to selectively remove persistent pollutants and high value products from water and wastewater streams.

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





Recent Publications

S. Habib and **S. T. Weinman**, A Review on the Synthesis of Fully Aromatic Polyamide Reverse Osmosis Membranes, *Desalination* 502, 114939 (**2021**).

S. Alipoori, H. Rouhi, E. Linn, H. Stumpfl, H. Mokarizadeh, M. R. Esfahani, A. Koh, **S. T. Weinman**, E. K. Wujcik, Polymer-Based Devices and Remediation Strategies for Emerging Contaminants in Water, *ACS Appl. Polym. Mater.* 3 (2), 549-577 (**2021**).

G. D. Barbosa, J. E. Bara, **S. T. Weinman**, C. H. Turner, Molecular Aspects of Temperature Swing Solvent Extraction for Brine Desalination Using Imidazole-Based Solvents, *Chem. Eng. Sci.* 247, 116866 (**2022**).

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Evan K. Wujcik

Advanced Materials, Wearable Electronics, Bio/Nanosensors, Polymers, Nanofibers, Electrospinning, Environmental Engineering

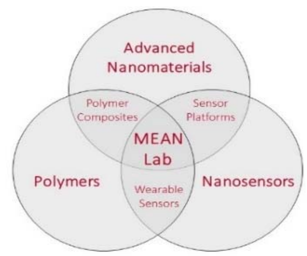
Evan K. Wujcik
Assistant Professor
PhD, Chemical & Biomolecular Engineering,
The University of Akron (2013)
M.B.A., The University of Rhode Island

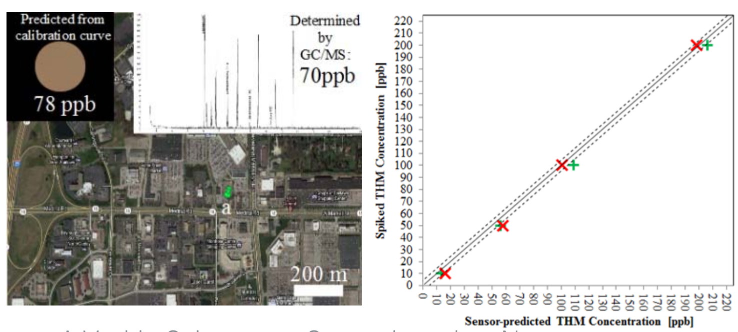
The **Materials Engineering And Nanosensor [MEAN] Laboratory** investigates and develops advanced materials, fundamental biomedical & environmental sensor platforms, and wearable electronics.

The MEAN Laboratory lies at the interface of materials science/ engineering, polymer science, nanotechnology, and surface (sensor)/interfacial science. From studying fundamental material properties and applications of nanomaterials comes innovative nanosensors, biosensors, wearable sensors, and bio-compatible materials applicable to a number of fields and disciplines.

College of Engineering
Chemical and Biological Engineering

Materials Engineering And Nanosensor [MEAN] Laboratory





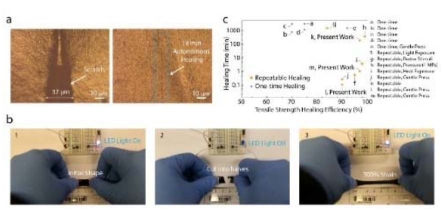
A Visible Colorimetric Sensor based on Nanoporous Polypropylene Fiber Membranes for the Determination of Trihalomethanes in Treated Drinking Water

Recent Publications

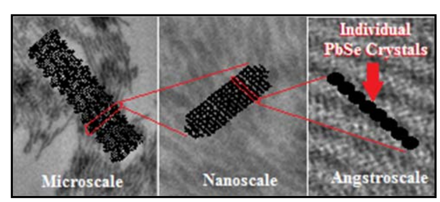
Y. Lu, Z. Liu, H. Yan, Q. Peng, R. Wang, M. E. Barkey, J. W. Jeon, **E. K. Wujcik,** Ultra-Stretchable Conductive Polymer Complex as Strain Sensor with Repeatable Autonomous Self-Healing Ability, *ACS Applied Materials & Interfaces* 11, 20453 (**2019**).

E. K. Wujcik, S. E. Duirk, G. G. Chase, C. N. Monty, A Visible Colorimetric Sensor Based on Nanoporous Polypropylene Fiber Membranes for the Determination of Trihalomethanes in Treated Drinking Water, *Sensors and Actuators B: Chemical* 223, 1 (**2016**).

Ultra-Stretchable Conductive Polymer Complex as Strain Sensor with Repeatable Autonomous Self-Healing Ability



Co-Electrospinning of Titania/Lead Selenide Nanostructures Organized Across Multiple Length Scales & Dimensions



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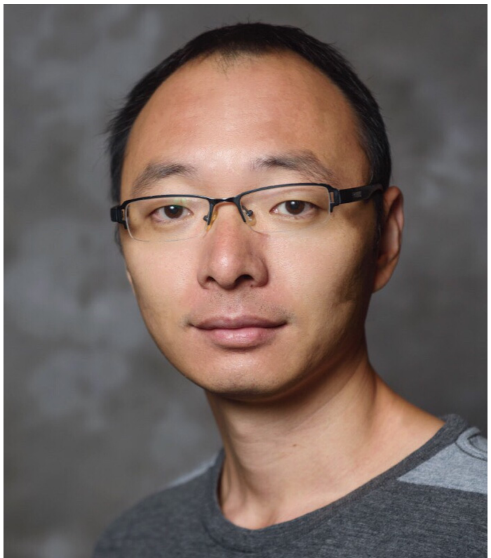
Chao Zhao

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, 2000776.* (**2020**).

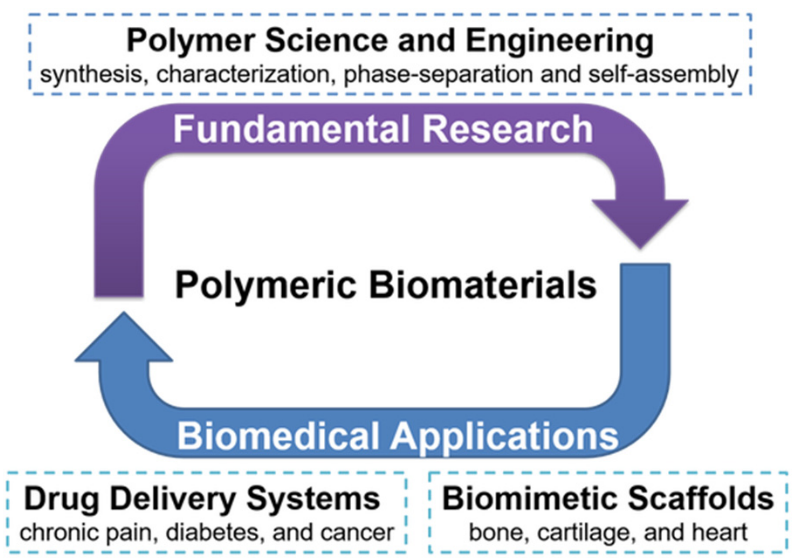
X. Li, Y. Zhao, **C. Zhao**, Applications of capillary action in drug delivery, *iScience*, 24(7):102810 (**2021**).

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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