

The Schoenborn Graduate Research Symposium & Exhibition

Department of Chemical and Biomolecular
Engineering
North Carolina State University

McKimmon Center
October 31st, 2022

Special thanks to:

The graduate student presenters

The Department of Chemical and Biomolecular Engineering

External judges:

Dr. Javier Grajeda (Eastman), Dr. Wes Bruce (BASF), and Dr. Preeta Datta
(Evonik)

Internal Judges:

Professors Gregory McKenna, Nathan Crook, and Jason Haugh

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Schoenborn 2022 Graduate Research Symposium

8:15 – 9:00 AM Continental Breakfast / Welcome

9:00 – 10:15 AM Oral Presentations Session I: Materials

- 9:00 AM **Sooik Im** *Enhanced Stability of Triboelectric Charge by Air-Stable Radicals*
- 9:15 AM **Sarah E. Morgan** *MOF-fabric for Chemical Warfare Agent Filtration: Journey from Toxic, Slow, Batch Synthesis to Benign, Rapid, Continuous Production*
- 9:30 AM **Fazel Bateni** *Intelligent Synthesis of Metal Halide Perovskite Nanocrystals Enabled by Modular Flow Reactors*
- 9:45 PM **Sunyoung Woo** *Creating Functional Surfaces with Tailorable Characteristics through Surface Attached Polymer Networks*
- 10:00 AM **Rachel S. Bang** *Multiphase Liquid Flow as a Universal Tool for Scalable Nanofabrication of Novel Polymer Morphologies*

10:15 – 10:45 AM Coffee Break

10:45 – 11:15 PM Oral Presentations Session II: Materials

- 10:45 AM **Yosra Kotb** *Novel High-Performance Sustainable Biopolymer Films Hierarchically Reinforced with Dendricolloids*
- 11:00 AM **Vahid Rahmanian** *Multifunctional Nanofibrous Aerogels: From 2D Hybrid Electrospun Nanofibers to 3D Self Supported Aerogels*

11:15 – 12:00 PM Oral Presentations Session III: Biotechnology & Biomolecular Engineering

- 11:15 AM **Eduardo Barbieri** *Potent Antibacterial Composite Nonwovens Functionalized with Bioactive Peptides and Polymers*
- 11:30 AM **Andrew S. Clark** *A bioinspired, microfluidic lobe filter for high throughput microparticle filtration*
- 11:45 AM **Jenna Meanor** *Comprehensive Mapping of the Histone Interactome*

12:00 – 2:15 PM Lunch

- 1:00 PM **Keynote Address: Dr. David Dudek, Western Digital**
Hard Disk Drives are Way Cooler Than You Think

2:15 – 4:00 PM Oral Presentations Session IV: Computational, Kinetics, and Catalysis

- 2:15 PM **Sudeep Sarma** *Designing Peptides Using Monte Carlo Search and Molecular Simulations for Diagnostic and Therapeutic Applications*
- 2:30 PM **Rakshit K. Jain** *Using Enhanced Sampling Simulations for Verification of the Improved CGenFF-NTOID Forcefield for Peptides*
- 2:45 PM **Leah Granger** *Modeling the Initiation and Propagation of Shock-Induced Damage in Crystalline Materials with Buried Interfaces*
- 3:00 – 3:30 PM **Coffee Break**
- 3:30 PM **Bradley A. Davis** *Intensified Fine Chemical Synthesis in Flow using Network-Supported Pd Catalyst*
- 3:45 PM **Junchen Liu** *Chemical Looping Oxidative Dehydrogenation of a Complex Alkylbenzene with Multifunctional Redox Catalysts*

4:00 – 6:00 PM Poster Session and Industrial Exhibit

Keynote Presentation

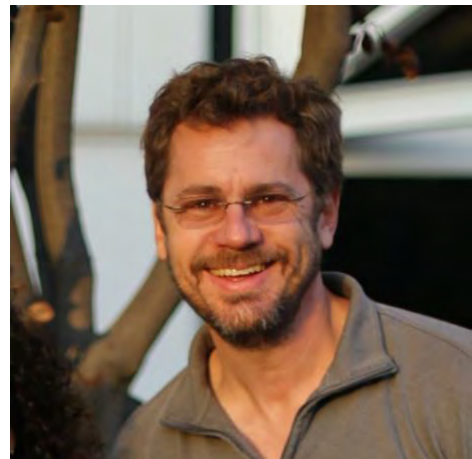
Hard Disk Drives are Way Cooler Than You Think – *Stories from a Typical NC State Ph.D., 23 Years After Joining the Company that Invented HDDs*

Dr. David Dudek

Director, Analytical and Characterization Engineering, Western Digital

Hard disk drives (HDDs) were invented in 1956. Since then, HDDs have evolved into incredibly complex devices containing a wide array of cutting-edge technologies, and the amount of information stored per surface area has increased by a factor of 500 million. The current status of this miniaturization process is a mechanical device in which the reading and writing head “flies” 75 mph at a distance of less than 10nm above a disk surface reading and writing 80-nm² bits of magnetic information onto media containing two dozen layers of thin films, some as thin as 10 Angstroms. An exceptional Analytical Sciences capability is required to support the advancement of HDD technology, the manufacture of heads and magnetic media (disks), the assembly of HDDs, and the diagnosis and prevention of failure mechanisms. Today’s talk will include (i) an overview of Western Digital’s world-class Analytical Sciences lab in San Jose, CA, (ii) a description of two particularly interesting HDD failure mechanisms, (iii) personal stories including how Dr. Dudek got his job, his career trajectory, and his management philosophy, and (iv) discussion of the one work-related thing he truly regrets, a story about a career-altering decision, and wrap up with a short list of unsolicited advice.

Biography: David Dudek (M.S. Management, ’97, Ph.D. Chemical Engineering, ’98) is a generalist and has a solid understanding of a large variety of analytical techniques as well as a large variety of manufacturing processes. He has been fortunate to tour manufacturing operations at Western Digital and WD-supplier factories on multiple continents. It is his great honor and privilege to be part of a team that works on materials-related challenges across Western Digital’s global business. He enjoys spending time (and traveling) with his wife (Naiomi, B.S. Chemical Engineering & B.S. Biochemistry ’95) and their three kids (aged 18, 16, and 13), playing ice hockey, and preparing and imbibing ethanol-containing beverages. He is currently Director, Analytical & Characterization Engineering, at WD’s Analytical Science lab in San Jose, CA, supporting the development, manufacture, and reliability of hard disk and solid-state storage devices.



List of Poster Presentations

Catalysis, Computation, and Kinetics

Matthew Dorsey (C1) *Computational Studies on the Structural Properties of Square Colloids with Offset Magnetic Dipoles*

Joseph Koelbl (C2) *Semi-deterministic phase field model predicts biased migration in haptotaxis*

Kevser Hilal Bektas (C3) *High throughput screening of redox-active perovskites and their applications in oxide-molten salt composites for ultra-high capacity thermal energy storage*

Aaron Frye (C4) *Chemical Looping Oxidative Dehydrogenation of Alkyl Benzenes with Multifunctional Redox Catalysts*

Mahe Rukh (C5) *Novel phase transition sorbents for isothermal sorption enhanced H₂ production*

Sherafghan Iftikhar (C6) *Mixed Oxides as Flexible Carriers for Tunable Syngas and CO₂ Utilization.*

William Martin (C7) *Tunable Syngas Production and Carbon Utilization via Ruddlesden Popper and Perovskite Catalysts*

Claire Murphy (C8) *Incipient Quantum Chemistry Calculations and Predicted Reaction Mechanisms for Incineration of Per- and Polyfluoroalkyl substances (PFAS)*

Materials

Man Hou Vong (M1) *Dewetting-Enabled Metal Oxides Exfoliation And Deposition From Liquid Metals*

Zvikomborero Machikiti (M2) *Controlling interfacial adhesion in polymer systems*

Jinge Xu (M3) *Autonomous Robotic End-to-End Synthesis of Metal Halide Perovskite Nanocrystals*

Shuang Jin (M4) *Reanalysis of an anomalous structural recovery in a polymer glass*

Prottasha Sarker (M5) *Regulating the rheology of collagen-based hydrogels using tannic acid particles*

Rami Awad (M6) *Self-Driving Fluidic Lab On Voyage to the Limits of the Nanomaterial Chemical Universe*

Jiangfeng Xu (M7) *Removal of phosphate using polyethyleneimine/poly(methyl vinyl ether-alt-maleic anhydride) hydrogels*

Hamed Morshedian (M8) *Accelerated In-Flow Photostability Studies of Quantum Dots*

Sneha Mukherjee (M9) *Paper Microfluidic Based Wearable Patches for Biomarker Sensing in Sweat*

Abhirup Basu (M10) *New classes of soft responsive magnetic microbeads by hierarchical assembly of nanoparticles confined in droplets*

Mesbah Ahmad (M11) *Novel biodegradable and stretchable films for soft electronics made of plasticized biopolymer composites*

Nidhi M. Diwakar (M12) *New Principles of Active Particle Propulsion Driven by Electrical and Chemical Gradients*

Haeleen Hong (M13) *Colloidal Design of New Types of Self-propelling Active Cleaners for Efficient Microplastics Remediation*

Fernando Delgado-Licona (M14) *Accelerated Multi-Stage Synthesis of Indium Phosphide Quantum Dots in Modular Flow Reactors*

Himendra Perera (M15) *Utilizing rheology to characterize carbon nanotube-polymer gels used in drag reduction applications.*

Nate Brown (M16) *Surface-initiated polymerization using gelatin-hydrogel reactors*

Mariam Sohail (M17) *Sustainable agrochemical sprays*

Lucille Verster (M18) *New Tools For Capture and Formation of Microplastics in Aqueous Environments*

Michael J. Petrecca (M19) *Applications of Soft Dendritic Colloids in Li-ion Batteries*

Sina Sadeghi (M20) *Smart Manufacturing of Metal Halide Perovskite Nanocrystals*

Biotechnology

Mahe Jabeen (B1) *3D model to study the invasion of extravillous trophoblast cells and interaction with stromal cells*

Zach Hetzler (B2) *Flexible Sensor Patch for Continuous Carbon Dioxide Monitoring*

Carly Catella (B3) *Developing therapeutic peptides against gastrointestinal pathogens for in situ treatment.*

John van Schaik (B4) *Maize Root Tool Kit*

Zidan Li (B5) *Inducible Directed Evolution of an Anticancer Terpene Biosynthetic Pathway in E. coli*

Tianyu Li (B6) *Engineering of Vibrio Natriegens for Degrading and Assimilating Poly(ethylene terephthalate) into Value-Added Products*

Z. Begum Yagci (B7) *An in vitro human platform to efficiently study Angelman Syndrome Class I/II deletion genes*

Kin Gomez (B8) *A study of Neurodegeneration: Beading patterns in C. elegans*

Ryan Bing (B9) *Extreme thermophily resists contamination and offers unique product separation opportunities for plant biomass fermentations*

Magdelene Lee (B10) *Characterization of solid-state DNA transfer for DNA-based Data Storage Systems*

Cyrus Cao (B11) *Information storage via immobilization of encoded DNA on ultra-high surface-area magnetic soft dendritic colloids*

Daniel J Willard (B12) *Life in Hot Acid: Exploring Key Mechanisms for Chemolithoautotrophy in Thermoacidophiles Through Comparative Phenotyping and Genotyping*

Mohamad Javad Haghghat Manesh (B13) *Biomining of Critical Metals Using Engineered Thermoacidophiles*

Ravikanth Appalabhotla (B14) *Deriving PLCy Single-Molecule Activation Statistics from Deterministic Simulations*

Abstracts for Oral Presentations

Enhanced stability of triboelectric charge by air-stable radicals

Sooik Im, Jan Genzer, Michael Dickey

Department of Chemical and Biomolecular Engineering, North Carolina State University

Background: Triboelectricity is a charging phenomenon when two materials are brought into contact and pulled apart. It was first discovered over two thousand years ago but remains poorly understood due to the stochastic nature of charges, making them hard to interpret [1]. One of the unclear issues in triboelectric charge is how the charges on the surface dissipate over time. So far, it is widely accepted that the charges on insulators decay naturally due to the breakdown caused by air and moisture, but the control of charge dissipation remains puzzled [2]. Preventing charge dissipation could enhance the efficiency of air filtration because the lifetime of charges is related to the ability to capture micro-sized particles on a filter media. Grzybowski et al. reported that charge decays faster after removing mechano-radicals generated from rubbing by a radical scavenger [3]. Based on the literature, radicals on the surface might be a key to enhancing charge retention. Still, to the best of our knowledge, no studies have reported on this phenomenon.

Results: Here, we investigated the role of air-stable radicals on charge retention with different self-assembled monolayers (SAMs) on Si wafers to find a way to enhance charge stability. Pt/Ti-coated atomic force microscopy probes were brought into contact with different SAMs to contact-charge the SAMs. The charge retention was recorded over time by the non-contact tapping mode of Kelvin Probe Force Microscopy (KPFM). The KPFM images showed that charges on hydrophilic surfaces generally tend to dissipate faster than those on hydrophobic surfaces, which indicates water vapor could enhance the charge dissipation. Interestingly, the charge retention in the presence of stable radicals (TEMPO) dissipated much slower (>12 h), showing out of the general trend. To verify the role of radicals in enhancing charge retention, radical density on the surface was tuned by two separate approaches: 1) treating TEMPO SAMs with tetrabutylammonium fluoride as a SAM etchant, and 2) using ascorbic acid as a radical scavenger. After these treatments, the charge destabilized by lowering radical density on the surface, confirming that the air-stable radicals could enhance the stability of triboelectric charges.

Conclusions: This study proposes new perspectives on increasing the retention of triboelectric charge by using air-stable radicals. Also, this new technique with KPFM will pave a new way to fundamentally characterize triboelectric charge, which is extremely difficult to analyze on a macro-scale.

References:

1. Lacks, Daniel, and Troy Shinbrot (2019). Long-standing and unresolved issues in triboelectric charging. *Nat. Rev. Chem.*, **3**: 465–476.
2. McCarty, Logan, and George M. Whitesides (2008). Electrostatic charging due to separation of ions at interfaces: contact electrification of ionic electrets. *Angew. Chem. Int. Ed.*, **47**: 2188–2207.
3. Baytekin, H. Tarik, Bilge Baytekin, Thomas M. Hermans, Bartłomiej Kowalczyk, and Bartosz A. Grzybowski (2013). Control of surface charges by radicals as a principle of antistatic polymers protecting electronic circuitry. *Science*, **341**: 1368–1371.

MOF-fabric for chemical warfare agent protection: journey from toxic, slow, batch synthesis to benign, rapid, continuous production

Sarah E. Morgan [1], Andie M. O'Connell [1], Morgan L. Willis [1], Carwynn D. Rivera [1], John J. Mahle [2], Gregory W. Peterson [2], Gregory N. Parsons [1]

1. Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, NC 27695; 2. U.S. Army Combat Capabilities Command Chemical Biological Center, Aberdeen Proving Ground, MD 21010

Background: Metal-organic framework (MOF) fabric composites have broad application in catalysis, viral remediation, gas separation, and toxin filtration. However, current synthesis approaches heavily rely on harmful solvents, long reaction times, and batch processing which all hinder process scalability and technology transfer. This work identifies a new, vapor-based route for MOF-fabric synthesis using environmentally conscious solvents, rapid reaction times, and industrially relevant semi-continuous processing. These advancements in technology readiness occurred over a multi-year journey including uncountable process iterations detailed in this synopsis. Our MOF-fabrics were developed for direct integration into chemical warfare agent protective gear due to their unique ability to adsorb and neutralize deadly organophosphate nerve agents.

Results: We first introduced a unique sorption-vapor synthesis (SVS) method of MOF-fabrics in which harnessed the inherent sorptive nature of polymers and vapor processing to substantially increase heterogenous MOF yield and limit homogenous MOF powder formation unavoidable in traditional approaches. Initial iterations relied on conventional harmful, high boiling point solvents including dimethylformamide (DMF).[1] Next, SVS was altered to use the bioderived, safe polar aprotic solvent γ -valerolactone (GVL) in replacement of DMF increasing sustainability but relying long reaction/ post processing times (> 72 h) and high process costs.[2] Further improvements replaced GVL with benign, low boiling point solvents significantly reducing cost, synthesis/ post processing times (< 2 h), and allowing adaption to semi-continuous processing of larger MOF-fabric swatches.[3,4] Advancements in synthesis methods were achieved in parallel with improvements in material functionality. Specifically, our state-of-the-art MOF-fabrics outperform the current protective standard activated carbon cloth in chemical warfare agent neutralization via hydrolysis and provide similar barrier properties.

Conclusions: The approaches outlined in this work present a scalable, rapid method for MOF-fabric production which is actively being improved by enlarging and refining semi-continuous methods along with regular testing of material performance. It is increasingly evident that the next generation of personal protective equipment is needed, and this work progresses advanced MOF-fabric technology closer towards warfighters and civilians living in turbulent regions.

References:

1. Morgan, S. E.; O'Connell, A. M.; Jansson, A.; Peterson, G. W.; Mahle, J. J.; Eldred, T. B.; Gao, W.; Parsons, G. N. (2021). *ACS Appl. Mater. Interfaces*, **13** (26), 31279–31284.
2. Morgan, S. E.; Willis, M. L.; Peterson, G. W.; Mahle, J. J.; Parsons, G. N. (2022). *ACS Sustain. Chem. Eng.*, **10** (8), 2699–27072.
3. Morgan, S. E.; Willis, M. L.; Dianat, Golnaz; Peterson, G. W.; Mahle, J. J.; Parsons, G. N. (in preparation)
4. U.S. Provisional Patent Application No. 63/279,923 filed on November 16, 2021

Intelligent Synthesis of Metal Halide Perovskite Nanocrystals Enabled by Modular Flow Reactors

Fazel Bateni [1], Sina Sadeghi [1], Venkat S. Punati [1], Christine Stark [1], Milad Abolhasani [1]

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Background: All-inorganic lead halide perovskite (LHP) quantum dots (QDs) have recently emerged as a promising class of semiconducting nanomaterials for a wide range of solution-processed photonic devices. Partial replacement of lead (Pb) cations with less toxic materials is considered an effective strategy to mitigate the toxicity of LHP QDs and impart new optical, optoelectronic, and/or magnetic properties into the pristine LHP QDs.[1] The synthesis, fundamental studies, and development of metal cation-doped LHP QDs are conventionally conducted using time-, material- and labor-intensive flask-based techniques.[1] Moreover, the discovery of optimal formulation and fundamental understanding of metal cation-doped LHP QDs are further limited by the manual nature of flask-based synthesis and characterization methods as well as the highly interdependent reaction and processing parameters in colloidal QD synthesis. The key to explore such a high-dimensional reaction space is through integration of the experimental platforms with artificial intelligence (AI)-assisted modeling and decision-making strategies to establish ‘self-driving’ laboratories.[2] Microfluidic reactors have shown great capabilities for establishment of closed-loop autonomous exploration and/or exploitation of the experimental space. Reduced chemical consumption and waste generation, reproducible and enhanced heat/mass transfer rates, and facile integration with in situ characterization techniques are the key factors to make a microfluidic platform an ideal tool for self-driven controlled synthesis of LHP QDs. [1,2]

Results: In this study, we studied the fundamental mechanisms of the colloidal synthesis, halide exchange, and cation doping of all-inorganic LHP QDs using a modular flow chemistry strategy. Building on this knowledge, we developed and integrated a multi-stage machine learning modeling and decision-making framework with the modular robo-fluidic QD synthesizer to achieve on-demand formulation optimization of LHP QDs with desired optical and optoelectronic properties for next-generation printed photonic devices.

Conclusions: We introduced, for the first time, an intelligent continuous flow platform for on-demand manganese (Mn) doping of cesium lead chloride (CsPbCl₃) QDs with a high degree of tunability through an in-flow cation-exchange reaction.[1] We systematically investigated the effect of dopant (MnCl₂) concentration and ligand composition on the kinetics, extent, and mechanistic aspects of the post synthetic cation-doping of LHP QDs. The developed self-driving laboratory using modular flow reactors enabled accelerated design space exploration, synthetic route discovery, and fundamental mechanistic studies of metal cation-doped LHP QDs.[2]

References:

[1] Bateni, F.; Epps, R. W.; Abdel-latif, K.; Dargis, R.; Han, S.; Volk, A. A.; Ramezani, M.; Cai, T.; Chen, O.; Abolhasani, M. Ultrafast Cation Doping of Perovskite Quantum Dots in Flow. *Matter* **2021**, S2590238521002174.

[2] Bateni, F.; Epps, R. W.; Antami, K.; Dargis, R.; Bennett, J. A.; Reyes, K. G.; Abolhasani, M. Autonomous Nanocrystal Doping by Self-Driving Fluidic Micro-Processors. *Advanced Intelligent Systems* **2022**, 2200017.

Creating functional surfaces with tailorable characteristics through surface-attached polymer networks

Sunyoung Woo [1], Jan Genzer [1]

1. Department of Chemical and Biomolecular Engineering, North Carolina State University

Background: The surface properties of polymers strongly affect many characteristics, such as wetting, antifouling properties, surface friction, or adhesion. The properties of surface anchored polymer, including polymer network at the interphase, are different from the bulk. The number of studies concerning such systems has increased in recent years. We used UV- or thermally-active cross-linkable groups to overcome the current limitations of generating substrate-anchored polymer networks. Using cross-linkable units reduces the fabrication steps and does not require special functional groups in polymers for cross-linking.¹

Results: To understand the mechanism and kinetics of surface anchored polymer network, we study the gelation of poly(vinylpyrrolidone) (PVP) network with various molecular weights and 6-azidosulfonylhexyl triethoxysilane (6ASHTES). PVP/6ASHTES mixture was deposited onto a silicon substrate by dip-coating and was annealed at 120, 130, and 140 °C for desired times. The gel fraction (P_{gel}) was determined as the change in film thickness before and after extraction of the polymer film. We established the time-temperature-composition relationship, which reveals that gel fraction can be adjusted by tailoring the amount of polymer, crosslinker, and experimental conditions. Additionally, the swelling behavior of the polymer network showed that the swelling ratio is proportional to the average molecular weight between cross-linking sites.² Next, we focused on the fabrication methods of a specific system that anchors an ex situ-forming hydrogel layer with commercial elastomers without physical modification. 4-azidosulfonylphenethyl trimethoxysilane (4ASPTMS) was rubbed on the elastomer surface and activated by annealing. Afterward, we placed a partially polymerized solution that acts as a precursor for depositing hydrogel. The resulting trilayer comprised elastomer-hydrogel-elastomer and was tested by a 180° peel test for the adhesion between the elastomer and hydrogel interface. Adding 4ASPTMS provided improved hydrogel adhesion to the elastomer and the hydrogel's water content affected the system's mechanical properties.

Conclusions: In this work, we investigated the kinetics of surface-anchored polymer networks using 6ASHTES. We studied gel fraction and swelling ratio to determine the effect of the polymer's molecular weight, annealing temperature, and time on the reaction kinetics of the surface-anchored polymer network. Furthermore, we proposed the fabrication method for hydrogel/elastomer laminates using chemical modification.

References:

1. Pandiyarajan, C. K., & Genzer, J. (2019). Thermally Activated One-Pot, Simultaneous Radical and Condensation Reactions Generate Surface-Anchored Network Layers from Common Polymers. *Macromolecules*, 52(2): 700-707.
2. Woo, S. Y., Pandiyarajan, C. K., & Genzer, J. (2021). Tuning the Properties of Surface-Anchored Polymer Networks by Varying the Concentration of a Thermally Activated Cross-Linker, Annealing Time, and Temperature in a One-Pot Reaction. *ACS Applied Polymer Materials*, 3(11): 5568-5577.

Multiphasic liquid nanofabrication of a multitude of soft matter morphologies

Rachel Bang [1], Sangchul Roh [1], Austin Williams [1], Orlin D. Velev [1]

1. Dept. of Chemical and Biomolecular Engineering, NC State University

Background: Many products used in modern-day society are composed of soft nanomaterials. Some applications include rheology modifiers, structural enhancers, nonwovens, and health care products [1]. Developing an efficient and scalable nanomaterial fabrication technique is crucial to improving productivity in both fundamental and applied technologies. Present conventional techniques can only produce a few morphologies such as particles, fibers, and rods. However, they may have low throughput and may not be capable of fabricating a wide range of structures or finer features. Our group has developed a versatile liquid shear-based nanofabrication technique that combines key concepts from nonsolvent-induced phase separation with interfacial polymer precipitation. During this process, a polymer solution is injected into a sheared bulk medium. The low miscibility between the polymer solution and the nonsolvent medium allows for extreme interfacial deformation by the fluid streamlines as the polymer precipitates [2]. Previously, we have shown that this method can produce rods and fibers in laminar flow and more complex dendritic structures and sheets in turbulent flows [2, 3]. Here, we present a systematic approach in determining the fabrication outcomes by developing a simple three-stage model.

Results: We focus our efforts on uncovering the fundamental mechanisms driving colloidal material fabrication. We developed a simple three-stage model that can effectively describe all possible operational conditions. The three stages consist of (1) Hydrodynamic shear, (2) Capillary stability and mechanical instability, and (3) Precipitation rate. When we divide the stages into two or three subcategories, we find twelve combinations of operational conditions which each produce a distinct colloidal morphology. Typically, laminar flows produce simple “one-dimensional” structures such as rods, fibers, and ribbons whereas turbulent flows can produce hierarchical structures similar to their multiscale vortices. The capillary stability primarily determines the jetting to the dripping transition of the injected polymer solution within laminar flows which drastically changes the outcome from fibers to spherical particles. The degree of mechanical entanglement in the precipitated polymer determines whether the polymer will undergo secondary fragmentation which can reduce their aspect ratios. The final stage concerns the precipitation rate which changes the timescale at which the polymer can be manipulated by shear.

Conclusions: Our systematic investigation into the liquid shear-based liquid manufacturing technique enabled the discovery and production of a plethora of novel colloidal morphologies. By simply varying the process conditions of the three operational stages, we have demonstrated that twelve structures with distinct morphologies can be made out of a single polymer. This technique is versatile and can be applied to many polymer systems for consumer products and new materials.

References:

1. Phillips, K. R. *et al.* A colloidoscope of colloid-based porous materials and their uses. *Chem. Soc. Rev.* **45**, 281–322 (2016).
2. Roh, S., Williams, A.H., Bang, R.S., Stoyanov, S.D., Velev, O.D. “Soft dendritic microparticles with unusual adhesion and structuring properties,” *Nat. Mater.*, **18**, 1315-1320 (2019).
3. Smoukov, S. K. *et al.* Scalable liquid shear-driven fabrication of polymer nanofibers. *Adv. Mater.* **27**, 2642–2647 (2015).

Novel High-Performance Sustainable Biopolymer Films Hierarchically Reinforced with Dendricolloids

Yosra Kotb [1], Orlin D. Velev [1]

1. Department of Chemical and Biomolecular Engineering, North Carolina State University

Background: The excessive production and use of petroleum-based plastics have created ominous environmental and ecological impacts, which is driving increased interest in developing biodegradable, renewable alternatives. Using natural biomass resources to develop alternatives to petroleum plastic films represents an attractive opportunity due to their abundance, low cost, and favorable biodegradability. However, these applications are still limited by their inferior mechanical strength and low stability against water. Here, we report a facile and sustainable method to reinforce polysaccharide films using a new class of dendritic colloidal particles [1,2]. These particles offer a nano- and microscale hierarchy to the films, as well as a network of hydrogen bonds, resulting in a remarkable increase in the mechanical properties and the wet film stability.

Results: Due to the high interfacial area, the large excluded volume, and van der Waals interactions, the soft dendritic colloids (SDC) have excellent structure building properties. We developed agarose biopolymer films reinforced with SDCs made of chitosan (CS), which is the second most abundant biopolymer in nature. The composite films showed synergistic functional properties due to the inclusion of CS SDCs, where the film's toughness showed a 4-fold increase compared to the pure agarose film. Due to intermolecular interactions between the biopolymers as well as nanoscale fibrous entanglement between the SDC, the films acquired a hydrophobic nature and an increased water stability. Other important film functional properties have also been characterized.

Conclusions: We have developed an all-natural, biodegradable film made from biopolymers that has superior or comparable properties to petroleum-based plastic films. The reinforcing based on SDC inclusion represents an innovative design strategy towards the fabrication of fully biodegradable and robust films that have integrated strength and toughness. The biopolymer film showed synergistic properties upon SDC addition in the matrix. We are currently investigating the fundamentals governing the intermolecular interactions between the film's components and the exact reinforcing mechanism.

References:

- [1] S. Roh, A.H. Williams, R.S. Bang, S.D. Stoyanov, O.D. Velev, Soft dendritic microparticles with unusual adhesion and structuring properties, *Nat. Mater.* (2019). <https://doi.org/10.1038/s41563-019-0508-z>.
- [2] O.D. Velev, Y. Kotb, Biodegradable Biopolymer Films, US Patent App. 17/584,569, 2022.

Multifunctional nanofibrous aerogels: From 2D hybrid electrospun nanofibers to 3D self-supported aerogels

Vahid Rahmanian, Tahira Pirzada, Saad A. Khan

Department of Chemical and Biomolecular Engineering, North Carolina State University

Background: From the first introduction of silica aerogel in 1930 to the most recent aerogels constructed from several organic and inorganic materials, design and fabrication of aerogels have been improved.^[1,2] Conventional aerogels are fabricated via solvent removal from a gelatinous network which is typically an expensive and time-consuming process. Additionally, conventional aerogels contain weak interconnected networks resulting in lack of mechanical flexibility and strength that inhibit their functionality. Recently, nanofibrous aerogels (NFAs) have started getting attention because of their straightforward and robust method of preparation. NFAs are prepared by freeze drying a dispersion of short nanofibers in a non-solvent.^[3,4] Synthesis of hybrid NFAs provide a flexible platform for creating functional materials from vast variety of organic and inorganic components. We present a sustainable approach to fabricate a mechanically robust and multifunctional aerogels from hybrid electrospun nanofibers.

Results: Ultralight ($\sim 10 \text{ mg cm}^{-1}$) and hierarchically porous ($> 99\%$) NFAs constructed from hybrid electrospun PVP-TiO₂ nanofibers and MOF decorated CDA-Silica nanofibers. Morphology of the aerogels analyzed using Scanning Electron Microscopy (SEM) and confocal laser scanning microscope while Energy Dispersive X-ray (EDX), X-ray Photoelectron Spectroscopy (XPS) and X-ray Diffraction (XRD) studies demonstrate a homogeneous distribution of TiO₂ and MOF particles in the structure of the aerogels. Owing to the photocatalytic activity of TiO₂, the PVP-TiO₂ aerogel exhibits antibacterial properties and VOCs and mineral oil decomposition. Additionally, we designed and developed MOF decorated CDA-Silica aerogel which has potential applications for filtration and CO₂ capture.

Conclusions: In this work, we have successfully developed a robust methodology to construct ultralight, hierarchically porous, mechanically strong, and multifunctional aerogels designed from hybrid electrospun nanofibers. As expected, in the PVP-TiO₂ aerogel, TiO₂ played an essential role in improving both the mechanical and functional properties of the aerogel. Crosslinking between TiO₂ and PVP is verified via appearances of Ti-O-C bands in the FTIR spectra of the hybrid fibers. On the other hand, MOF decorated CDA-Silica aerogel designed with potential applications for filtration and CO₂ capture. These on-demand attributes of our hybrid NFAs together with its inherent mechanical resilience and thermal insulation render it a viable material platform for potential use in diverse applications.

References:

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Potent Antibacterial Composite Nonwovens Functionalized with Bioactive Peptides and Polymers

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Background: Antimicrobial-resistant infections (AMRs) are responsible for more than 35,000 deaths in the USA and 700 000 deaths worldwide annually.^[1,2] Development of new materials that deliver antimicrobial agents to pathogenic microorganisms offers a path to reducing AMRs. In this context, nonwoven fabrics (NWFs) are an ideal platform for delivering antimicrobial agents, ubiquitous in environments with a higher risk of bacterial contamination, such as hospitals and clinics.^[3] Therefore, this project aimed to investigate strategies to incorporate antibacterial peptides and polymers on NWF substrates.

Results: We modified polyethylene terephthalate (PET) NWFs by covalently conjugating polyethyleneimine (PEI) followed by adsorption of daptomycin or anionic polymer polyacrylic acid (PAA) for loading of polymyxin B. The PET/PEI NWFs showed loading of 0.3 µg of daptomycin per mg of NWFs and 3.2 log reduction of *S. aureus*. In comparison, PAA/PEI/PET NWFs displayed 1.1 µg of polymyxin B per mg of NWFs and at least 4.2 log reduction of *E. coli*. In a second approach, different formulations of poly(*N*-isopropyl acrylamide-*co*-2-aminoethyl acrylamide-*co*-2-guanidinoethyl methacrylamide) P(NIPAM-*co*-AEMA-*co*-GUMA) or poly(NIPAM-*co*-methacrylic acid-*co*-2-hydroxyethyl acrylate) P(NIPAM-*co*-MAA-*co*-HEA) microgels were crosslinked on PET or polypropylene (PP) NWFs by activation of P(NIPAM-*co*-4-benzoylphenyl-acrylamide) under UV light. We confirmed coating NWFs with P(NIPAM-*co*-AEMA-*co*-GUMA) or microgels by gravimetric analysis and scanning electron microscopy (SEM). The selected formulations of P(NIPAM-*co*-AEMA-*co*-GUMA) PP and PET NWFs showed more than 5 log reductions of *S. aureus* and *E. coli*. We detected a fast release of peptide bacitracin from microgels without HEA (>90% released in <2 days), and slow release from microgels with a high mole fraction of HEA (60% of bacitracin released after 3 weeks). Bacitracin or polymyxin-loaded microgels on NWFs reduced bacterial concentration by more than 5 logs after 3-hour contact.

Conclusions: We developed scalable methods to produce antibacterial fabrics by functionalizing nonwoven fiber mats with antimicrobial peptides and polymers. Polymer-based coatings and microgels were utilized to adsorb antibacterial peptides. Fabrics with sustained release of bacitracin and polymyxin showed a 100,000-fold reduction of *S. aureus* and *E. coli* in artificial sweat with no adverse effect on human skin cells.

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A bioinspired, microfluidic lobe filter for high throughput microparticle filtration

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Background: Inertial microfluidics aims to overcome downfalls from typical sieve filtration, such as clogging, by offering continuous separation using only passive, hydrodynamic forces that arise in microchannels [1]. However, since inertial particle separation depends highly on flow rate, separation efficiencies are limited to explicit flow rates – too high or too low and particle separation will not occur. Interestingly, the Manta Ray’s non-clogging filter feeding mechanism relies on inertial particle separation. When swimming speeds increase, zooplankton deviate from the fluid streamlines and continue their inertial path. Importantly, feeding efficiency does not decrease at higher flow rates [2]. In this work, we develop a microfluidic microparticle filter bioinspired by *M. tarapacana*’s filter lobe structure that is capable of filtering 10-30 μm particles with flow rates up to 20 mL/min in a single device.

Results: We fabricated a microfluidic lobe filter bioinspired by *M. tarapacana* that features two arrays of filter lobes separated by 46 μm along with one inlet and two outlets. Particle suspensions of 10-30 μm particles at $\sim 10^6$ part/mL were inserted into the filter at various flow rates ranging from 0.5 mL/min to 20 mL/min. As expected, slow inlet speeds resulted in low filtration efficiencies with the largest particle sizes experiencing the highest efficiencies. Once inlet flow rates topped 4 mL/min, particles with sizes over 20 μm obtained high efficiencies over 90%. As inlet flow surpassed 6 mL/min, 20-30 μm particles’ filtration efficiency effectively plateaued. At 10 mL/min, the 20-25 μm particle size range obtained peak efficiency of 98% and the 25-30 μm bin obtained a peak efficiency of 99.5%. Moreover, both the 10-15 μm and 15-20 μm bins obtained peak efficiencies of 85% and 95%, respectively. We used ANSYS Fluent simulations to explain the separation phenomena. These simulations revealed complex velocity profiles with inflection points within the main channel of the device. In the region between the local velocity maxima nearest the lobe array and the inflection point, the inertial lift force will change directions [3]. We hypothesized that comparing particle size (D_p) to the distance from the lobe array to closest local velocity maxima (U^*) and inflection point (D^*), would provide an explanation to lobe filtration success. For instance, if $D_p > D^*$, efficient filtration would be achieved. Remarkably, simulation-derived filtration efficiency estimates matched well with experimental filtration efficiencies.

Conclusions: Microfluidic lobe filtration, bioinspired *M. tarapacana*, offers high throughput microparticle filtration for 10-30 μm particles at processing speeds of 20 mL/min. Comparing the distances from the lobe array to the velocity profile’s local maxima and inflection point to a particle’s diameter provides a simple, yet robust explanation for filtration success.

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Comprehensive mapping of the histone interactome

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Background: In the cell, DNA exists in a highly compact state to fit in the nucleus. The main structure of DNA are chromosomes which can be further broken down into nucleosomes: DNA wrapped around an octamer of histone proteins to form a “beads on a string” structure [1-3]. The interaction between DNA and these histone proteins directly affects many diverse cellular functions. Histone proteins undergo small chemical changes which can alter the histone protein structure and by extension, gene expression [1-3]. Detecting histone modifications and characterizing their binding interactions are crucial to further our understanding of chromatin biochemistry and gene regulation. Unfortunately, due to the complex nature of histone proteins, it has proven difficult to use classic protein engineering platforms. High-throughput platforms could accelerate work in this field and could also be used to engineer novel affinity reagents towards histone modifications.

Results: We have determined specific experimental conditions that affect binding specificities of post-translationally modified histones in classic protein engineering platforms. These findings have been used in developing a yeast surface display platform in which a library containing 200+ natural histone binding proteins has been created and that can be used in one-pot mapping of histone-protein interactions, directed evolution studies to engineer new histone binding proteins, and importantly be the first system that can efficiently map both the interactome and affinities simultaneously in high throughput of histone-protein interactions.

Conclusions: Histone peptides do not follow conventional rules when used in traditional protein engineering platforms. Histone tails have high charge density, low hydrophobicity, and are intrinsically disordered. Altering avidity in separation strategies through soluble peptide labeling is able to rescue the specificity of these binding interactions. Applying these conditions to our yeast surface display platform we report both the binding specificity and affinities of 200+ human histone binding proteins to over 30 distinct histone modifications, bioinformatically identify common features and ontological families through clustering analyses, and discuss the impact of this new interactome on our understanding of human gene regulation and disease. Included in the library of histone binding proteins are cancer-linked mutants, and we also identify the effect of these mutations on binding affinity and specificity.

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Designing Peptides Using Monte Carlo Search and Molecular Simulations for Diagnostic and Therapeutic Applications

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Background: The design of multifunctional peptides on the computer to address challenges in health and technology has advanced in recent years, with the maturation of computational algorithms and the protein database. We have developed an efficient *Peptide Binding Design* algorithm (PepBD) that employs a Monte-Carlo search in peptide sequence and conformation space to discover peptides that bind with high affinity and selectivity to specific biomolecular targets. The performance of the best peptide binders predicted by PepBD is evaluated *in-silico* by performing atomistic molecular dynamics simulations and calculating binding free energies. Our peptides are experimentally tested *in-vitro* in binding and cell-based assays.

Results: We have used our computational peptide design strategy to discover peptides that bind to (1) SARS-CoV-2 Receptor Binding Domain (RBD) and inhibit SARS-CoV-2 cell entry; and (2) *C. diff.* toxin A with the aim of neutralizing *C. diff.* toxicity in large intestinal cells. In **Project 1**, we use a 23-mer peptide, SBP1, as the reference peptide. SBP1 is derived from the peptidase domain of ACE2 (Angiotensin Converting Enzyme 2), the human host receptor that the SARS-CoV-2 virus uses for cell entry. Our *in-silico* peptide, P4, binds to the Wuhan-Hu-1, Kappa, and Delta strain of the SARS-CoV-2 RBD with micromolar level affinity, as measured using a tryptophan fluorescence quenching assay but cannot outcompete ACE2 in a competitive ELISA assay.¹ (2) In **Project 2**, we discover an 8-mer peptide, SA1, that binds to the *C. diff.* toxin A glucosyltransferase domain (GTD). The efficacy of peptide SA1 was tested using a trans-epithelial electrical resistance (TEER) assay on monolayers of the human gut epithelial culture model. Peptide SA1 blocks TcdA toxicity in jejunum (small intestine) cells and in colon epithelial cells, and exhibits a binding affinity, K_D , of 56.1 ± 29.8 nM as measured by surface plasmon resonance (SPR)^{2,3}.

Conclusions: Our computational peptide design algorithm enables us to rapidly discover peptide binders with high affinity and selectivity for biomolecular targets. The iterative procedure examines as many as ~50,000 peptide sequences. We describe two projects. In **project 1**, we discover an ACE2-derived peptide, P4, that binds to the SARS-CoV-2 RBD with micromolar level affinity but cannot inhibit ACE2:SARS-CoV-2 interaction, and, in **project 2**, we discover an 8-mer peptide, SA1, that binds to *C. diff.* Toxin A GTD with nanomolar level affinity and neutralizes *C. diff.* toxicity in jejunum and in colon cells. Peptide P4 and SA1 are promising candidates for diagnostic and therapeutic applications respectively.

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Using enhanced sampling simulations to improve the CGenFF-NTOID forcefield for peptoids

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Background: Peptoids, or poly N-substituted glycines, are synthetic biocompatible peptidomimetics that have been used to develop antimicrobial agents, lung surfactants and drug delivery vehicles. They are protease resistant and have enhanced cellular uptake, which further make them attractive candidates for biological applications. Since peptoids lack native backbone hydrogens connected to an electronegative atom, and hence have no backbone hydrogen bonding, their secondary structure is governed primarily by steric interactions (in the absence of specific interactions between side chains). Furthermore, unlike peptides, which have trans configuration as the prevalent amide bond isomer, peptoid amide bonds can have both cis- and trans- configurations. This allows peptoids to exhibit a variety of secondary structures that are not observed in peptides. Due to these differences and the varied accessible secondary structures between peptoids and peptides, force fields fitted for peptides have very limited applicability for peptoids. Weiser and Santiso [1] recently developed an atomistic force field for peptoids, NTOID, which is based on CGenFF. They displayed that NTOID is capable of modeling peptoids with amide bonds in both the cis- and trans- conformation for three different sidechain residues. In this work, we present an extension of this approach so as to increase the applicability of the developed NTOID model.

Results: Recently, an online utility known as the Peptoid Data Bank [2] has been developed, which stores experimental structural and XRD crystallographic data for peptoids. Using an application of the utility, we were able to determine which sidechain residues to consider next, based on the number of papers published focusing on each of them. This pointed us to two residues, N-(methoxyethyl) glycine and (S)-N-(1-naphthylethyl) glycine. The parameters for these sidechains were optimized using enhanced sampling simulations in the software package NAMD while fitting to the structural preferences observed in solution.

Conclusions: The newly developed parameters, coupled with the 3 already fitted sidechains to the forcefield, allows us to study a large number of polypeptoid chains through simulations and analyze the secondary structures and the associated folding mechanisms.

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Modeling the initiation and propagation of shock-induced damage in crystalline materials with buried interfaces

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Background: Reactive inorganic nanolaminates contain metastable interfaces, such as those between metals and metal oxides, that when disturbed by heat or shock undergo highly exothermic reactions. Largely due to the potential complexity of the system dynamics and the challenges associated with experimental probes of the dynamics at buried interfaces, the mechanisms that initiate this chemistry are unknown. We use atomistic molecular dynamics simulations of nanolaminates to investigate the mechanisms by which the energy of a shock pulse – delivered by a simulated flyer plate – can initiate and propagate damage at a buried interface.

Results: Our simulations using the embedded atom method on FCC Cu/Ni bilayers show dislocations initiated at the edges of the flyer plate and propagating downward along slip planes. The propagation and behavior of the shock-induced damage depend on the energy of the flyer plate, which in this case is controlled by the initial velocity. Low-velocity impacts result in transient damage in the upper layer; in addition to defects originating at the flyer plate perimeter, the interaction of the compression wave with interfacial defects initiates additional dislocations that travel upward. High-velocity impacts result in plastic damage in both layers, where damage in the upper layer also slips along the interface while the damage in the lower layer appears to be a result of compression directly under the flyer plate. We further investigated the shock-induced damage using the Ackland algorithm [1] to determine local lattice structure and the dislocation extraction algorithm [2] to visualize specific types of line defects. Within each FCC layer, Shockley partial dislocations are most common and surround regions of atoms with a local HCP structure, indicating the presence of stacking faults. Additional partial defects emerge as dislocations interact with each other and interfacial defects.

Conclusions: The presence of the observed defects appears to relieve the shock-induced stresses. The crystallographic orientation and the energy delivered by the flyer plate affect the depth of damage observed as well as whether damage is reflected or travels through an interface. Our simulations indicate the mechanisms by which energy is delivered across a series of buried interfaces may differ depending on the interface location with respect to the shock pulse. This work was supported by the U.S. Department of Defense, Multidisciplinary University Research Initiative through the Army Research Office, Grant No. W911NF-16-1-0406.

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Intensified Fine Chemical Synthesis in Flow using Network-Supported Pd Catalyst

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Background: Metal-mediated chemical reactions have been a crucial area of research for over a century. Recent efforts aim to increase metal-mediated catalysis's performance by optimizing the structure and chemical environment of active catalytic species towards process intensification and sustainability. Network-supported catalysts use a solid support with embedded metal catalysts, ideally allowing for efficient precursor access to the catalytic sites and simultaneously not requiring a catalyst separation step following the reaction.¹

Results: Integrating the unique advantages of network-supported catalysts and flow chemistry, we have developed a cartridge-like flow reactor for continuous synthesis of fine chemicals with high efficiency and catalyst reusability. First, we investigated using a silicone elastomer, poly(methyl hydrosiloxane) (PMHS), as the catalyst support.² The Si-H units on the PMHS backbone act as the crosslinking site and the reducing agent to anchor and reduce palladium, Pd (II) acetate to Pd (0). The PMHS-supported Pd catalyst was packed into a stainless-steel flow reactor for the continuous operation of a model Suzuki-Miyaura cross-coupling reaction. We systematically investigated the role of reaction temperature, catalyst loading, crosslinking density, and gel particle size on the transient and steady-state behavior of the cartridge-like flow reactor. The PMHS-supported catalytic particles demonstrate minimal deactivation and leaching over a continuous (80 h) Suzuki-Miyaura cross-coupling reaction at a 30 min nominal residence time at 95°C. Next, we investigated using azide-functionalized β -cyclodextrin as the catalyst support. The resulting network facilitated the addition of coordinated Pd nanoparticle growth, resulting in a robust and stable catalyst for continuous hydrogenation of nitroarenes. The synthesized catalytic particles were packed in a flow reactor to manufacture aryl amines under mild conditions continuously. The Pd-cyclodextrin polymer network demonstrated yields of >99% for the selective hydrogenation of 19 different nitroarenes in a 1-min residence time. The developed catalyst was reusable across many substrates and solvents; it was used to study a two-step telescopic reaction to synthesize an intermediate for the antibacterial drug Linezolid. Both network-supported catalysts provided low catalyst deactivation over multi-day runs with no detectable leaching under reaction conditions.

Conclusions: The developed flow chemistry platform was utilized for two network-supported catalysts for continuous Pd-catalyzed chemical transformations. The PMHS/VTEG polymer network improved catalytic performance and activity as a continuous, ligand-free C-C cross-coupling catalyst. The Pd-cyclodextrin polymer network catalyst was highly effective for chemoselective hydrogenation of nitroarenes and provided distinct benefits over traditional methods of producing aryl amines.

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Chemical Looping Oxidative Dehydrogenation of a Complex Alkylbenzene with Multifunctional catalysts

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Background: meta-Diisopropenylbenzene (m-DIPEB) is an important precursor for cross-linked polymers and resins [1]. Compared to other similar structured monomers such as styrene, m-DIPEB has a smaller demand but is of higher value. Therefore, an energy-efficient and highly selective process is required to make it economical.

Results: We report a redox oxidative dehydrogenation (R-ODH) process to produce DIPEB from m-diisopropylbenzene (m-DIPB) based on a La-Ca-Mn-O@K-Fe-O catalyst. The catalyst can convert m-DIPB to m-DIPEB with K-Fe-O phase while selectively oxidizing the dehydrogenation by-product H₂ with La-Ca-Mn-O *in-situ*. This oxidative approach could circumvent the conventional dehydrogenation conversion limitation while supplying heat to the catalytic reactor, achieving an m-DIPEB single-pass yield of 75%, which represents a >100% increase to the conventional process. An Aspen Plus® simulation indicate that the proposed process has the potential to reduce energy requirement by 72%. X-ray photoelectron spectroscopy and X-ray fluorescence indicate the K concentration near-surface is ~110% higher than the bulk concentration, suggesting the formation of a core-shell structure. *in-situ* XRD indicate that the KFeO₂ phase was formed during the ODH reaction, and La-Ca-Mn-O acts as the sacrificial phase to prevent KFeO₂ from reducing by H₂ and KFeO₂. Del-plot method suggests that the DIPEB could form via two routes: 1) m-DIPB → m-isopropenylcumene → m-DIPEB (sequential); 2) m-DIPB → m-DIPEB (concerted) [2].

Conclusions: In summary, we reported a La-Ca-Mn-O@K-Fe-O core shell catalyst which exhibit 75% yield towards m-DIPEB. As a result, ~72% energy requirement reduction can be achieved. X-ray characterization techniques confirm the core-shell structure of the catalyst, and that the core acts as a sacrificial phase to maintain catalytic KFeO₂. Kinetic experiments suggest the reaction route process via both sequential dehydrogenation and concerted dehydrogenation route.

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Abstracts for Poster Presentations

Computational Studies on the Structural Properties of Square Colloids with Offset Magnetic Dipoles

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Background: In recent work, Velev and coworkers have developed a new class of engineered materials that interact, assemble, reconfigure, and propel in response to external magnetic and electric fields [1]. Cubic microparticles with a ferromagnetic-metallic coating on one or two opposing faces retain residual polarization when exposed to an external magnetic field, even after the field is turned off. The many different interactions that exist when anisotropic, magnetically-polarized colloidal particles are placed in tunable, external fields creates numerous design variables that are challenging to fully explore experimentally. The search for potentially useful structures formed by this colloidal material can be enhanced by computer simulations of colloidal assembly. In this work, we used Discontinuous Molecular Dynamics (DMD) to simulate the behavior of large systems of dipolar squares in the absence of a magnetic field. DMD is a fast variant of standard molecular dynamics that is applicable to systems of molecules interacting via discontinuous potentials, and is best suited for exploring phenomena that occur at long time scales. Microcubes were represented in quasi-2D as groupings of hard discs bonded together to create a rigid square geometry. Magnetic dipoles were mimicked *in silico* by embedding opposite electrostatic charges along one cubic face. Annealing, or “slow-cooling”, simulations were performed in the absence of a magnetic field using the model described above to discover the equilibrium conformations of the dipolar squares.

Results: We find that, as the strength of the dipolar interactions between squares overcomes the system’s thermal energy, the dipolar squares assemble into single- or double-stranded assemblies, each with unique structures and phase diagrams in the temperature-density plane. Single-stranded assemblies of dipolar squares are associated with the formation of a percolated, or gel-like, state, while double stranded assemblies are associated with the formation of a nematic state. Using pairwise potential energy calculations between dipolar squares, we show that whether a system of dipolar squares assembles into single- or double-stranded conformations depends on how the dipole is embedded within the square. Furthermore, by parameterizing the location of the dipole within the square, we predict that certain dipolar squares can transition between percolated and nematic states, depending on the system’s density.

Conclusions: Our results highlight how colloidal particles with several degrees of anisotropy exhibit a rich phase behavior that sensitively depends on particle geometry and directional interactions. Our theoretical predictions are useful to colloidal scientists that are attempting to rationally synthesize particles with controllable properties. Finally, our studies of dipolar squares in the absence of a magnetic field provide a useful background as we extend our simulations to dipolar squares in the presence of an external magnetic field.

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Phase Field Model to Study Integrin Based Signaling and Fibroblast Haptotaxis

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Background: When invading a wound, skin cells called fibroblasts are presented with an array of different directional cues. Among the directional cues, gradients of immobilized ligands found in the extracellular matrix are understudied yet thought to be critical for invasion. Recent publications show an importance of lamellipodia and integrin-actin machinery in migration toward these surface bound ligands, called haptotaxis [1]. Considering the initial literature on the haptotactic response of fibroblasts a 2-D haptotactic migration model was developed to mimic fibroblast migration with integrin signaling.

Results: A finite volume PDE solver (Virtual Cell) was used to implement stochastic adhesion networks with prescribed biases to exponential haptotactic gradients. Cells, modeled according to the phase field formalism, are superimposed onto the adhesion gradients. A simple signaling and protrusion response to the adhesion networks is meant to reflect integrin based signaling important to haptotaxis and causes translocation of the phase field cell. The current model causes significant deformation and translocation of the phase field cells and biased migration in relative gradients greater than 5%.

Conclusions: Preliminary results of the model show that in high gradients cells behave similarly to what is seen in experimental fibroblasts on fibronectin gradients. These results are promising as these initial iterations are toy models that at their basic level still grasp some biological relevance. Later model iterations would hope to capture membrane and protrusive forces and integrin based signaling in a more descriptive way.

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High-throughput screening of redox-active perovskites for ultra-high-capacity thermal energy storage

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Background: Industrial activities represent a major source for greenhouse gas emissions through the combustion of fossil fuels. As a result, they also release large amounts of waste heat [1]. Recovery of waste heat provides an excellent opportunity to boost energy efficiency and reduce environmental impacts [2]. The main challenge in the use of industrial waste heat is the mismatch between the time and operating temperature requirement of heat release and heat demand [2]. Low-cost energy storage technologies that can store large amount of heat within a tailorable operating temperature range can address this challenge. Recently, redox-active perovskites have exhibited the capacity for ultra-high performance thermochemical energy storage via O₂ release/uptake within tailorable temperature swings (400-1000°C). The operating temperature window, heat release capacity and O₂ release capacity can be tuned for waste heat recovery by varying the types and ratios of A- and/or B- site dopants. We aim to optimize the perovskites in terms of their thermodynamic properties by utilizing a DFT based model that provides us with the high-throughput computational screenings of Sr_{1-x}A_xFe_yB_{1-y}O₃ perovskites.

Results: Since the studies on in the literature is very limited, our main focus has been developing a family of Sr_{1-x}A_xFe_yB_{1-y}O₃ perovskites candidates for TES. Among 2003 screened materials, we selected 209 promising candidates to experimentally investigate by considering their O₂ capacity, enthalpy and material cost. We synthesized 60 of them, measured O₂ release capacity for 40 samples (the ones with pure perovskite phases) and enthalpy for 17 of them. Ba-based perovskites exhibited superior O₂ redox capacity in 400-800 °C while Ca-based perovskites exhibited superior O₂ redox capacity in 800-1100 °C. In the B-site, increasing the ratios of Mg and Ti adversely affected phase purity or O₂ capacity. A-site dopant types and ratios were found to affect O₂ capacity more than B-sites. Ca-doped and La-doped samples achieved higher enthalpy values than Ba-doped ones. A Ca and Mn-doped SrFeO₃ material exhibited the highest ΔH of 160 kJ/mol O. Energy density up to 67 kJ/kg_{ABO₃} at 400-800 °C in air was also achieved. Our experimental results showed DFT model had better predictions of ΔH and ΔG for the samples with larger O₂ release capacity and 65% of the predicted data were within 30% deviation.

Conclusions: We determined the promising candidates among Sr_{1-x}A_xFe_yB_{1-y}O₃ perovskites that can be used in oxide-molten salt composites. We demonstrated that despite of its limitations, DFT model can be used as an efficient tool for the optimization of perovskites for TES applications.

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Chemical Looping Oxidative Dehydrogenation of Alkyl Benzenes with Multifunctional Redox Catalysts

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Background: Alpha-Methyl Styrene (AMS) is an important comonomer in many polymerization processes which improve the material's impact and heat resistance [3]. AMS and similar alkenyl benzene compounds are conventionally produced from endothermic catalytic dehydrogenation which suffers from yield limitations and high energy requirements [2]. An energy efficient and high single pass yield is desired to improve the economics of AMS production.

Results: We report an alternative redox oxidative dehydrogenation (R-ODH) process to produce AMS from cumene utilizing a family of Ca-Mn-O@K-Fe-O catalysts. The catalytically active K-Fe-O shell converts cumene to AMS while the oxygen carrying Ca-Mn-O-based core donates lattice oxygen to selectively oxidize the hydrogen byproduct in-situ. This approach fundamentally shifts the reaction equilibrium by oxidizing the hydrogen byproduct, achieving an AMS single pass yield of 58.7%. Additionally, the selective hydrogen oxidation supplies heat to the catalytic reactor, enabling reduced energy consumption as compared to conventional dehydrogenation. Aspen Plus simulations suggest that this process could reduce the energy requirement to produce AMS by >50%. Ex-situ X-ray diffraction (XRD) indicates the formation of CaMnO₃ perovskite and mixed K-Fe-O phases. X-ray fluorescence (XRF) and X-ray photoelectron spectroscopy (XPS) confirm the presence of a potassium-rich shell, supporting the core-shell nature of the catalyst. In a previous study [1], in-situ XRD indicates that the catalytically active KFeO₂ phase forms during the reaction while the Ca-Mn-O core acts as the sacrificial reduced phase to prevent KFeO₂ reduction.

Conclusions: The Ca-Mn-O@K-Fe-O core-shell redox catalyst reported can achieve 58.7% yield of AMS from cumene. The fundamental change to selectively oxidize the hydrogen byproduct shifts the reaction equilibrium towards AMS, as well as reducing the energy requirements by >50%. The catalyst characterization techniques performed illustrated the sacrificial behavior of the catalyst core, as well as confirmed the presence of a catalytically active KFeO₂ shell.

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Novel phase transition sorbents for isothermal sorption enhanced hydrogen production

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Background: The sorption-enhanced steam reforming (SESR) technology capitalizes on the in-situ removal of CO₂, which shifts the thermodynamic equilibrium of the water-gas shift reaction in favor of producing an H₂ stream with enhanced yield and purity. CO₂ sorbents commonly used in the SESR process can be classified into the following categories: CaO-based sorbents, alkali-metal sorbents, hydrotalcite sorbents, and bifunctional/trifunctional materials in which sorption and catalytic sites are mixed in microscale. However, sintering at high temperatures, slow kinetics, mass and heat transfer limitation, and high pCO₂ requirement deem as disadvantages for such sorbents. From a process point of view, mostly the temperature swing process has been adopted in which the heat exchange and entropy generation in the heating and cooling steps accounts for more than 80% of the total cycle. In contrast, an isothermal adsorption-desorption cycle will minimize the exergy loss. Our proposed perovskite structure-based phase transition sorbents (Sr_xCa_{1-x}Fe_yCO_{1-y}O₃) can be reduced and regenerated to different phases in isothermal conditions due to large non-stoichiometry and redox activity. The reduced metal oxide phases formed during the reforming stage are responsible for CO₂ capture and shift the equilibrium of WGS for more H₂ production. Hence, it is imperative to understand the driving force for such phase transitions that enable cyclic carbonation and regeneration. The best performing PTS (phase transition sorbent) from our screening showed ~45 mol% CO₂ sorption from 10 vol% CO₂ streams in the preliminary TGA experiment which has 60 mole% Sr on the A-site and 70 mole% Co on B-site. In-situ XRD has confirmed the phase change behavior of the sorbents at 750°C triggered by varying partial pressure of oxygen. The thermodynamic analysis and experimental studies performed confirmed that changing pO₂ would trigger carbonation or decarbonation at a given pCO₂ and sorption performance depends on the reducibility of the PTS. Moreover, the thermodynamic analysis will facilitate the design of PTS to meet specific H₂/syngas yields.

Mixed oxides as flexible carriers for tunable syngas and carbon utilization

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Background: CO₂ is a major contributor to global climate change. Current CO₂ utilization technologies are energy intensive[1]. In addition, the design of solid catalysts for CO₂ utilization still relies on heuristics and trial and error[2]. Therefore, cost-effective CO₂ capture and utilization technologies, as well as effective computational tools to narrow down the design space for solid catalysts for CO₂ utilization are highly desirable. Greenhouse gases such as CO₂ and CH₄ can be converted to syngas (a mixture of CO and H₂) which is an important feedstock for many industrially important chemicals that require various ratios of H₂ to CO. Therefore, flexible materials that can accomplish such a task are highly desirable as well.

Results: In the present work, various schemes such as chemical looping methane partial oxidation/cracking/reforming (CLPOx/CLMC/CLMR) are explored for the tunable production of syngas via mixed oxides serving as oxygen, carbon, and CO₂ carriers respectively. The specific oxide compositions for CLPOx, i.e. Sr_{0.625}La_{0.375}Fe_{0.625}Ti_{0.375}O_{3-δ}, Sr_{0.5}Sm_{0.5}Fe_{0.625}Ti_{0.375}O_{3-δ}, Sr_{0.625}Y_{0.375}Fe_{0.5}Ti_{0.5}O_{3-δ}, and LaFe_{0.375}Mn_{0.625}O_{3-δ} were selected on DFT-based materials screening, which identified perovskite oxides with optimal equilibrium oxygen partial pressure (P_{O_2}) for CO₂-splitting and methane partial oxidation. Experimental investigations corroborated well with the predictive redox performance of redox catalysts (RCs). Impregnation of the RCs with 1 wt.% ruthenium (Ru) was found to be highly effective to enhance the reaction kinetics specifically for 1wt% Ru/LaFe_{0.375}Mn_{0.625}O₃ which showed >90% CO₂ conversion and >85% methane conversion with ~95% CO selectivity at 800 °C. In addition, we also found that LaFe_{1-x}Ni_xO₃ serves as flexible oxygen or carbon carriers for tunable syngas production and CO₂ utilization where CH₄ and CO₂ conversions varied between 85% and 98%, and 70–88%, respectively. While H₂/CO ratio from Fe-rich redox catalysts was ~2.3:1 in the methane conversion step, Ni-rich catalysts produced a concentrated (~ 93.7 vol%) hydrogen stream via methane cracking. In addition, we also found that the strontium-based Ruddlesden-Popper and Perovskite phase-based mixed oxides serve as flexible oxygen or CO₂ carriers for the tunable production of syngas where >80% CH₄ conversion and >90% CO₂ utilization was observed.

Conclusions: In conclusion, we report mixed oxides with excellent redox properties that not only produce tunable syngas ratios by utilizing carbon but also the carbon/oxygen/carbon dioxide carrying ability of various mixed oxides allows carbon dioxide utilization under a wide range of carbon dioxide concentration in the feed. These findings would ultimately allow chemical industries to minimize carbon emissions and produce valuable feedstocks (syngas) for chemical production.

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Tunable Syngas Production and Carbon Utilization via Ruddlesden-Popper and Perovskite Phase-Based Catalysts

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Background: Syngas is a useful commodity to produce industrially important chemicals. Dry reforming of methane (DRM) offers the opportunity to produce syngas by utilizing CO₂, however, DRM is a highly endothermic process and the co-feeding of CO₂/CH₄ requires further processing to obtain pure syngas [1]. To address this, we propose a sorbent looping dry reforming of methane (SLDRM) and a chemical looping partial oxidation of methane (CLPOx) scheme for the tunable production of syngas via the use of Ruddlesden-Popper (RP) and Perovskite (PV) phase-based catalysts respectively. Advantages of a SLDRM over a typical DRM scheme is that by partitioning CO₂ and CH₄ into two separate steps, SLDRM offers the combination of both capture/conversion, which lowers the energy intensive process of capture, and has the flexibility of utilizing a variety of feedstocks that contain CO₂ [2].

Results: The general chemical structure of RP and PV is best described as the following: A_{n+1}B_nO_{3n+1} (1 ≤ n < ∞) where if n = 1 then it is RP and as n increases to infinity it will exhibit a PV phase. As n increases, the functionality of the catalyst changes from a CO₂ carrier to a O₂ carrier. A-site dopants include Sr and La where B-site dopants include Fe and Cu/Ni. Cu/Ni lower the activation energy of CH₄ and CO₂ for conversion, La provides the support to allow dispersion of Cu and Ni (confirmed through TEM), Sr acts as the support but also acts to form carbonates, and Fe assists lattice oxygen transport within the catalyst. After 20 redox cycles at 900°C, all catalysts exhibit >80% CH₄ conversion as well as >90% CO₂ utilization, whereas PV catalysts exhibit <5% CO₂ capture and RP exhibit >60%. A tunable H₂/CO ratio is also achieved with RP catalysts by varying the reforming/carbonation time. *Ex-situ* XRD was able to show clear distinctions between the RP and PV catalysts of the same composition of elements and *in-situ* XRD was able to show the formation of carbonates during the carbonation step for RP catalysts. CO₂ capture can be dictated by the molar ratio of Sr/Fe, where an increased ratio (RP) leads to increased CO₂ capture. Interchanging Cu as the B-site dopant increases CO₂ capture to as high as 90% (H₂/CO ≈ 1) but presents issues of deactivation due to sintering of Cu, whereas the use of Ni has minimal deactivation and has CO₂ capture as high as 60% (H₂/CO ≈ 1.3).

Conclusions: In conclusion, we report a relatively stable family of catalysts that can serve a function of tunable H₂/CO production as well as efficient carbon utilization. RP and PV serve similar purposes of tunable syngas production, but their applications are different depending on the process upstream. Catalyst deactivation was rather minimal and through a SLDRM scheme, we can have flexible catalysts with dual functionality.

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Early Quantum Chemistry Calculation Results and Predicted Reaction Mechanisms for Incineration of Per- and Polyfluoroalkyl substances (PFAS)

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Background: Once widely used in fire-fighting applications because of their superior performance, aqueous film-forming foams (AFFF) containing PFAS now present environmental and public health hazards [1]. The effectiveness of fluorine-containing compounds is attributed to their resistance to destruction. However because of this inability to degrade, PFAS lingers in the environment and bioaccumulates. Incineration of PFAS-containing AFFF is thought to be the most effective route for safe destruction and disposal [3]. We are working with the EPA to develop PFAS incinerators and require accurate rates of PFAS destruction and formation of products of incomplete combustion (PICs). The EPA is testing pilot-scale incineration via their Rainbow Furnace at their EPA/RTP campus. We are using quantum chemistry to develop reaction mechanisms and collaborating with the EPA to verify results.

Results: Our overall research objective is establishing the reaction kinetics of four PFAS-surrogate small-chain compounds: perfluoro-octanoic acid (PFOA), perfluoro-octanesulfonic acid (PFOS), and potassium perfluorocarboxylate salts of PFOA and PFOS. To date, we have modeled the gas-phase combustion of PFOA. In a computational context, the number of electrons is quite large (because of the presence of fluorine). Here we report initial B3LYP/6-31G(d,p) model chemistry results. There are three main destruction pathways observed: pericyclic decomposition, homolytic scission, and hydrogen abstraction. Fluoroalkyl radicals are created from hydrogen abstraction (initially just 1H-perfluoroalkanes + R•) and then rapid CO₂ scission within perfluorooctanoate. The fluoroalkyls can then β-scission with an activation energy of 38 kcal/mol. The perfluoroalkanes are generally stable, but homolytic scission can still occur along the C-C bonds.

Conclusions: A first pass at gas-phase combustion kinetics modeled via computational quantum chemistry and reaction theory has produced reasonable activation energies in agreement with literature available. Higher-level calculations are ongoing in CBS-QB3 as well as calculations for condensed-phase destruction of PFOA and are expected to produce more accurate results. In future work, kinetics data will be derived from quantum chemistry calculations and used to simulate incinerator conditions for comparison to experimental data.

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Dewetting-Enabled Metal Oxide Exfoliation & Deposition from Liquid Metal

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Background: Amorphous gallium oxide (GaO_x) is a wide bandgap, transparent semiconductor. Because of its optical transparency and deep ultraviolet (DUV, $\lambda=200\text{-}300\text{nm}$) light absorption, it has been proposed as a promising material for optoelectronics in literature.[1] The bandgap energy and carrier mobility of GaO_x can also be tailored by alloying with other metallic cations (i.e, indium) or creating oxygen vacancies, which further enable its applications in digital memory and transistors.[2,3] Such metallic doped- and undoped- GaO_x thin films are typically synthesized via conventional physical or chemical vapor deposition; However, the long process usually requires undesirable toxic gas precursors, elevated temperatures, and a vacuum environment. A recent, novel approach to obtain metal oxide or alloy oxide thin films is to exfoliate the native oxides of liquid gallium or its alloy metals (LMs). Similar to most metals, LMs – a class of metal with a melting temperature close to room temperature – reacts readily with oxygen in air and forms a thin oxide ($\sim 3\text{nm}$) on the surface under ambient condition.[4] Despite the advantage of attaining metal oxide and alloy oxide thin films in ambient conditions using LMs, most proposed techniques in current literature can only synthesize/deposit continuous metal oxides films in small area with minimal LM residues ($<20\text{ cm}^2$).[4] Herein, we proposed a technique to continuously exfoliate and deposit large area ($>60\text{ cm}^2$) GaO_x and amorphous gallium indium oxides (GaInO_x) films ($\sim 3\text{nm}$ in thickness) from their host LMs.

Results: Large area GaO_x and GaInO_x exfoliations from LM were demonstrated by inducing continuous dewetting of LMs, called “dewetting-enabled continuous metal oxides printing” (DECMOP). The exfoliated GaO_x and GaInO_x films were characterized using optical microscopy, EDS/TEM, XPS, and TOF-SIMS. Specifically, the optical microscope images showed the area of the deposited oxides ($>60\text{cm}^2$) and their color difference before and after annealing. The cross-sectional images of the GaO_x and GaInO_x were captured using TEM. The cross-sectional TEM images were also used to determine the thickness of the oxides ($\sim 3\text{nm}$). The chemical mapping from EDS/TEM confirmed the presence of GaO_x and GaInO_x . The chemical compositions of the printed oxides and its depth profile were obtained using XPS and TOF-SIMS respectively.

Conclusions: Our results showed that DECMOP is a viable, low-cost method to deposit large area GaO_x or GaInO_x thin films onto substrates at ambient conditions. This work also provides insights of the wetting/dewetting mechanism of LMs.

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Reducing polymer/polymer interface adhesion to facilitate fracture

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Background: Interfacial adhesion is a fundamental property of interest in bicomponent polymer fibers. The interfacial adhesion ranges from weak to strong depending on the polymer pair. The chemical bonds between polymer pairs directly influence interfacial adhesion strength, which in turn impacts the surface structure, mechanical properties of fibers, and material performance. Here, the bicomponent polymer systems tested are poly(ethylene terephthalate) (PET)/nylon 6 (PA6), polypropylene (PP)/PET, polyethylene (PE)/PA6, polylactic acid (PLA)/PP, nylon 66 (PA66)/PET, nylon 11 (PA11)/PET, and nylon 12 (PA12)/PET. These pairs exhibit distinct levels of mutual adhesion at various temperatures due to chemical bond formation. Therefore, we are developing an understanding of the variation of adhesion in different polymer systems while tailoring the adhesion at the PET/PA6 interface by adding modifiers that react preferentially with the PA6 component. We study the adhesion strength of bicomponent polymer systems. We examine the feasibility of modifying a polymer pair system using the modifiers, *i.e.*, poly(styrene-alt-maleic anhydride) (PSMA) and poly(octadecene-alt-maleic anhydride) (POMA). We assess the impact of varying functional group concentrations on the adhesion strength between nylons and PET.

Results: The lack of compatible functional groups in a bicomponent polymer system results in weak adhesion between the polymers, as evidenced in the PP/PET, PP/PLA, and PA6/PE systems. The adhesion strength in the nylons/PET systems showed that PA66/PET had the highest adhesion energy, followed by PA6/PET, PA11/PET, and PA12/PET. Polymer pairs were also found to display higher adhesion at elevated temperatures and longer annealing times. PA6 reacts with PSMA and POMA, and both modifiers reduce interfacial adhesion strength between PET and PA6.

Conclusions: Overall, we established strong adhesion between polymer pairs because of the possible strong chemical interactions between the functional groups. In the nylons/PET systems, we saw that the nylons with the highest concentration of available amines had the strongest adhesion with PET as more chemical bonds formed. PA6 modified with POMA had a more significant reduction in adhesion strength in a PA6/PET system than PA6 modified with PSMA. The “C18 motif” present in POMA may block ester (in PET) and/or secondary amines (in PA6), thereby decreasing adhesion strength.

Self-Driving Robotic Researcher: End-to-End Synthesis of Metal Halide Perovskite Nanocrystals

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Background: Perovskite quantum dots (PeQDs) have recently emerged as a promising candidate for printed clean energy technologies. Rapid growth of ionic PeQDs is due to their unique optical properties that cannot be obtained from bulk scale, including near-unity photoluminescence quantum yields (PLQYs), narrow emission spectra, broad absorption spectra, and facile bandgap tunability [1]. Even with the proven potential of PeQDs in devices, understanding their formation mechanism and precision synthesis remain a challenge. Despite the critical role of both surface ligands and antisolvents on the structural integrity and properties of PeQDs [2], the field currently lacks a detailed understanding of the effect of these intertwined parameters on the synthesis science of PeQDs. This knowledge gap can be attributed to the exponentially growing size of the experimental space that needs to be explored for synthesis and purification of PeQDs (exceeding 10^8 potential number of experiments), and the time-, labor-, and resource-intensive nature of the current manual experimentation techniques. Herein, we present a self-driving robotic researcher to investigate the underlying formation mechanism of PeQDs in the presence of different surface capping ligands combined with an antisolvent-based purification.

Results: The self-driving robotic researcher uses a modular robotic synthesis and purification platform guided by a modular artificial intelligence (AI)-assisted modeling and decision-making framework to navigate through the multivariate high-dimensional design space of PeQDs. Cesium lead bromide (CsPbBr_3) QDs were used as an exemplary PeQDs to develop the self-driving robotic researcher. Butyric Acid, Hexanoic Acid, Octanoic Acid, and Oleic Acid were used as the starting surface ligand libraries of CsPbBr_3 QDs (*i.e.*, the discrete parameters). The autonomous robotic QD synthesizer was able to rapidly identify the surface ligand and anti-solvent resulting in the best-performing QD (*i.e.*, the highest purification yield with the highest photoluminescence quantum yield, PLQY, for a given peak emission wavelength) with minimum experimental cost (minimum number of experiments).

Conclusions: The developed self-driving robotic researcher was capable of automated precursor preparation, synthesis, and purification of colloidal nanomaterials integrated with real-time absorption and photoluminescence characterizations. Bayesian Optimization facilitated the navigation through the multivariate high-dimensional design space of PeQDs and rapidly identified the best-performing surface ligand and antisolvent in a time-, labor-, and resource-efficient manner. The robotic researcher discovered that a long alkyl chain surface ligand and a moderate polarity antisolvent resulted in the highest PLQY and purification yield of CsPbBr_3 QDs.

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The problem of temperature error: revisiting the anomalous structural recovery in a polymer glass

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Background: In the isothermal structural recovery of polymer glass, the departure from equilibrium is generally viewed as smooth functions of time as shown in the dilatometric studies by Kovacs [1]. However, recent studies by Boucher et al. [2] and Cangialosi et al. [3] reported two mechanism structural recovery in enthalpy at aging temperatures ranging from 6 to 17 K below T_g of polystyrene, drawing considerable interest. In an attempt to replicate the results, Koh and Simon [4] conducted one-year isothermal aging experiments on polystyrene of similar molecular weight at 15 K below T_g , and did not observe the intermediate plateau in the two-mechanism structural recovery. There remains important work to determine what could cause the non-smooth structural recovery.

Results: In this study, we test the hypothesis that poor temperature control that is typical of a vacuum oven could lead to the anomalous results. We use Tool-Narayanaswamy-Moynihan (TNM) model to calculate the structural recovery of polystyrene undergoing such thermal histories that were affected by the vacuum oven temperature variation and find that the reported two mechanism structural (enthalpy) recovery can be reproduced when such temperature variability was considered.

Conclusions: In conclusion, we have proposed the hypothesis that the unexpected intermediate plateaux in the structural recovery data reported by Cangialosi et al. [3] arise due to small errors in the aging temperature applied to the samples by examining the details of experimental procedure. The TNM model calculation for a set of hypothetical thermal histories shows that small temperature errors up to 3 K difference between the actual T_a and set temperature, possibly due to the temperature drift inside the DSC because of frost buildup and spatial and temporal variability in temperature inside the vacuum oven, could be the plausible explanation for the anomalous plateaux in the reported work.

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Rheology of collagen-based hydrogels tailored by tannic acid particles

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Background: Hydrogels are porous three-dimensional structures composed of polymeric cross-linked networks that has the provision for sufficient water and nutrient flow for cell proliferation to stimulate the regeneration of defective tissues. Compared to surgical scaffold implantation, injectable hydrogels can be easily applied by minimal invasive techniques to form a self-standing hydrogel. Naturally derived polymer, collagen, has been widely employed as injectable hydrogel since it inherits the structural and functional cursors to accelerate tissue formation, however it shows poor rheological properties. The use of biodegradable tannic acid particles provides a useful approach to improve the rheology of these systems while its inherent antibacterial and anticarcinogenic nature adds to gel functionality. Polyphenolic tannic acid particles could potentially interact with collagen through their hydroxyl and carboxyl groups allowing us to modulate the rheology.

Results: In this study, we examined how liquid as well as particulate tannic acids impact the rheological properties of collagen-based hydrogels. Liquid and needle-shaped tannic acid particles are synthesized and incorporated into collagen in this regard. While samples exhibit solution-like features at storage conditions (4°C), they transform into gels under physiological temperatures (37°C). The sol-gel transition in terms of temperature and time is monitored as a function of tannic acid concentration. Interestingly, particulate tannic acid incorporation exhibits the largest increase in elastic modulus with shape playing a secondary factor. Measurement of yield stress using the elastic stress method also reveals a similar trend. These results are interpreted in terms of the underlying interactions of tannic acid with collagen, as probed by spectroscopy. Importantly, compared to neat collagen hydrogels, those containing TA microparticles show similar cell viability (human dermal fibroblasts) and comparative cellular activity.

Conclusions: The use of needle-shaped tannic acid particles provides a facile approach to control the rheological characteristics of collagen hydrogel. In particular, changes in microstructure and cross-linking kinetics leads to hydrogels with enhanced modulus and yield stress while still preserving injectability. Results from this work could lead to the development of a new functional hybrid hydrogel system for use as injectables in tissue regeneration technology

Self-Driving Fluidic Lab On Voyage to the Limits of the Nanomaterial Chemical Universe

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Background: Nanoparticles are important for our daily life activities due to their rapidly growing applications in energy, sustainability, and healthcare sectors. The nature of precursor chemistries as well as process parameters effect structure, shape, and size, and in turn the nanoparticle's specific functions and applications. Thus, very precise synthesis is needed to achieve the desired physicochemical properties of nanoparticles. Precision synthesis is difficult using manual batch synthesis techniques due to batch-to-batch variation and slow and irreproducible mass and heat transfer rates. Exploring the vast intrinsic and extrinsic parameter space of nanoparticles to find their optimal synthetic route for the targeted properties is also laborious and expensive using batch reactors due to large reagent consumption and experimentation times. Recent advancements of reaction miniaturization, online characterization techniques, and data science tools, provide an exciting opportunity to digitize nanoparticle synthesis. In this work, we present a machine learning-guided fluidic robot to accelerate nanoparticle discovery and development. Nanoparticles synthesis can be controlled more precisely with microfluidics due to automation and fast and controllable heat and mass transfer rates. Machine learning modeling and decision-making under uncertainty assist with exploring the vast nanoparticle synthesis space efficiently and intelligently to rapidly identify the synthetic route that results in the desired properties in as few experiments as possible, saving time and resources. [1]

Results: The functionality of the developed self-driving fluidic lab is assessed through Pareto front mapping of all-inorganic metal halide perovskite quantum dots (QDs) that shows the best combination tradeoffs of photoluminescence quantum yield PLQY (efficiency in emitting light) and full width at half maximum FWHM (measure of color quality) that can be attained for any peak emission energy E_p (color) of the QDs. The QD precursors are mixed sequentially, sent to a heated flow reactor to synthesize the cesium lead halide QDs, and then characterized online *via* a flow cell to acquire UV-Vis absorption and photoluminescence spectra. The spectra are further processed to calculate the PLQY, FWHM, and E_p of the in-flow synthesized QDs. An ensemble neural network is used as the surrogate model to map the reaction temperature, residence time, lead to cesium ratio, bromide to iodide ratio, and concentration to the PLQY, FWHM, and E_p . The model is updated iteratively after each experiment in a closed loop and is used with Bayesian optimization to find the conditions with maximal hypervolume improvement to map the Pareto front with minimum number of experiments.

Conclusions: The Pareto front of QDs was mapped autonomously with minimum cost, thereby accelerating the discovery of and finding the chemical universe limits of metal halide perovskite QDs, despite their process sensitive nature. The self-driving fluidic lab presented here has the potential to accelerate discovery of colloidal nanoparticles beyond the ones studied here, with its modularity allowing for further modifications of the system.

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Phosphate removal by poly (methyl vinyl ether-alt-maleic anhydride)-polyethylene imine networks

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Background: Eutrophication has elicited numerous problems worldwide, including decreasing species diversity. We are seeking to find a low-cost and convenient way to meet the phosphate concentration limit in the water bodies.

Results: Branched polyethylene imine (PEI) precipitates at low concentrations (<100 mg/L) with phosphate anions and with heteropoly-molybdenum blue (HMB) under acidic conditions. This method is promising for phosphate capturing. We further form hydrogels by reacting PEI with poly (methyl vinyl ether-alt-maleic anhydride) (PMVEMA). The PMVEMA-PEI hydrogels absorb phosphate efficiently with HMB at pH=2 and release phosphate at pH=11. The gel system could also detect the presence of phosphate with a noticeable color change, from colorless to blue. Finally, we examine the stability of PMVEMA-PEI hydrogels from pH=2 to pH=12. We use infrared spectroscopy (IR) to characterize the PMVEMA-PEI hydrogels before and after phosphate adsorption.

Conclusions: PMVEMA-PEI hydrogels are confirmed to show great capability of capturing phosphate under acidic conditions. They can also be applied to detect the phosphate with heteropoly-molybdenum blue.

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Accelerated In-Flow Photostability Studies of Quantum Dots

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Background: Quantum dots (QDs) are colloidal semiconductor nanocrystals with size-tunable bandgaps and unique optoelectronic properties such as high quantum yields, narrow emission linewidths, and high light absorption cross-sections. Such characteristics make QDs an attractive class of materials for a wide range of applications, including optoelectronic devices, bio-imaging, and photo-catalysis. Every application of QDs involves their exposure to photons. Therefore, photostability studies of QDs are considered a critical step in their research and development. Nevertheless, evaluating the photostability of QDs with the common flask-based methods is very time-consuming and suffers from variations in the experimental conditions, leading to irreproducible results. Microscale flow reactors, with their reduced light absorption path lengths compared to batch reactors, can significantly accelerate the QDs' photostability studies *via* enhancing the irradiant photon flux.

Results: This work presents an automated single-droplet microfluidic platform for accelerated photostability studies of colloidal QDs. During each experiment, a 10 μL droplet of QDs — three orders of magnitude smaller than the typical flask-based experiments — was oscillated back and forth in a photochemical reactor illuminated by a collimated UV light source with a precisely tunable photon flux. The oscillatory flow reactor made it possible to decouple the residence time and the flow rate, thereby maintaining the mixing rate inside the droplet constant regardless of the residence time. The UV-Vis absorption and photoluminescence (PL) spectra of the QDs were automatically recorded at each oscillation cycle, *in-situ*, using a custom-designed flow cell. Specifically, we used cadmium selenide (CdSe) QDs as a testbed of the developed platform. The effect of the initial average size of CdSe QDs on their photostability was studied by conducting experiments on QD samples with different PL peak wavelengths. Next, the effect of photon flux was evaluated by conducting photostability experiments using different collimated UV powers. It was observed that the photo-oxidation reaction, occurring at the surface of CdSe QDs, resulted in etching the nanocrystals (supported by a blue shift in their peak emission wavelength) and reducing their concentration. Photo-oxidation can either decrease the quantum yield of QDs by creating new surface trap states or temporarily increase the quantum yield by passivating the existing surface traps [1]. We discovered that the overall photo-degradation rate is greater for the QDs with smaller initial sizes as they possess higher surface-to-volume ratios. Also, the overall photo-degradation rate increases with increasing the photon flux.

Conclusions: One of the most important yet challenging to study characteristics of QDs is their photostability. The developed modular microfluidic platform in this work enabled rapid photostability studies of colloidal QDs in a precisely controlled microenvironment. The results of this study can guide the design of surface-engineered QDs with the long-term photostability required for their adoption by printed energy technologies.

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Paper Microfluidics Based Wearable Patches for Biomarker Sensing in Sweat

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Background: The monitoring of human health and well-being with the use of wearable devices is the core of the next generation of biomedical devices. Sweat provides a facile source for the continuous and non-invasive measurements of biomarkers. Despite its advantages, sweat biomarker analysis is still challenging because most of the commercially available health-monitoring devices are either semi-invasive in nature (iontophoresis) or operate only during active sweating. Our team has introduced a simple and efficient platform for sweat sampling and handling based on osmotic-capillary principles and paper microfluidics. It can harvest sweat noninvasively without the necessity of active perspiration.[1] The patches use three robust physical effects: osmosis, capillary wicking, and evaporation. Osmotic sweat withdrawal is achieved by interfacing the skin with a hydrogel disk containing concentrated solute. The extracted sweat is transported on a paper strip via wicking and disposed on an evaporation pad. Here, we will discuss how these principles were applied in the development of a class of simple and inexpensive wearable skin patches for analysis of potassium, lactate, and cortisol, based on lateral flow assays (LFAs).

Results: Our LFA platform is composed of silicone, a paper microfluidic conduit attached to a commercial K^+ strip, and a polyacrylamide hydrogel with a higher osmotic strength than sweat. *In-vitro* testing on gelatin-based model skin (pre-infused with known quantity of K^+ ions) allowed calibrating the platform with model sweat. Human trials revealed that it can function with very low sweat volumes ($\sim 2\text{-}3\ \mu\text{L}$) and can detect K^+ levels from human skin under moderate intensity exercise and rest. We also observed that sweat K^+ levels are independent of the sweat rate and proportional to blood. The patch could also efficiently sample sweat lactate directly from the surface of skin. On-skin testing of the platform on both resting and exercising human subjects confirms that the patch can extract sweat and analyze the changing lactate levels. The results show that lactate in sweat increases with exercise and as a direct result of muscle activity. Concurrently, we are working on interfacing the paper platform to electrochemical sweat lactate sensors, where the enzymatic electrodes are printed on the paper strip that continuously transports the sweat from the hydrogel-skin interface towards the evaporation pad. This will allow long-term continuous electronic readout of the results from the wearable interface. We are also developing wearable skin LFAs for detection of cortisol (in sweat) as a key stress biomarker in individuals, soldiers in combat, athletes, and emergency personnel.

Conclusions: The non-invasive wearable patches that we have developed can enhance affordable advanced healthcare, by eliminating the need to visit medical centers for biomarker-based diagnostics. These simple, facile, and inexpensive patches could allow numerous opportunities for at-home or in-field POC diagnostics.

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New classes of responsive soft magnetic microbeads by hierarchical assembly of nanoparticles confined in droplets

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Background: Directed assembly of colloidal particles using magnetic field serves as a facile method for creating hierarchical structures. Upon applying a magnetic field, paramagnetic particles acquire magnetic dipoles and align themselves to form varied architectures, ranging from linear to higher-dimensional arrangements depending on the intensity and direction of the magnetic field. While the assembly of magnetic nanoparticles (MNPs) assisted by magnetic field in infinite geometries has long been established, little is yet known about how these particles interact in confined geometries. In the current study, directed assembly of iron oxide nanoparticles inside microdroplets of sizes ranging from 2 to 25 μm by using a static magnetic field was investigated. Liquid polydimethylsiloxane (PDMS) precursor embedded with MNPs was dispersed in a shear-thinning fluid to synthesize the microdroplets with randomly distributed nanoparticles. The controlled assembly of the MNPs was achieved by applying an external magnetic field, and then the microdroplets were crosslinked to form soft PDMS microbeads with embedded aligned nanoparticle structures.

Results: By changing the MNP concentrations from 1.25 wt% to 10 wt%, we discovered structural phase transitions inside the PDMS beads ranging from disconnected short chains to 2D linear chains to 3D networked bundles. It was found that below a critical microbead size, the MNPs did not align to form chains, and then the number of chains increased with the increase in the size of the PDMS microbeads. We established correlations between the number of chains formed inside the beads with the cross-sectional area of the beads. The number of chains increased linearly with the microbead size; interestingly, the number of chains remained almost constant till bead cross-section of 100 μm^2 and then decreased with increase in MNP concentration. Instead, the average cross-sectional area per unit chain was found to increase from 0.83 μm^2 to 8.39 μm^2 as the MNP concentration was increased from 1.25% to 5%, which supported the increase in the hierarchy of the assemblies from disconnected chains to 3D bundles. Our experimental findings have been further supported by COMSOL simulation results which showed how the magnetic energy changed as the conformations of the chains were changed within a microbead of a specific size.

Conclusions: The soft magnetic microbeads that will be synthesized in large amounts could find applications in new responsive gels, 3D printed soft actuators, active particles, biomedical formulations, and novel drug delivery techniques. They enable a broad range of fundamental research in new metamaterials assembly.

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Novel biodegradable and stretchable films for soft electronics made of plasticized biopolymer composites

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Background: Soft electronics is becoming widespread all over the world having wide range of applications such as robotics [1], medical field [2], and defense [3]. However, introduction of these electronics is posing new perils to the environment mainly due to accumulation of electronic waste. Introducing of sustainable biodegradable materials can largely eliminate this problem. Since substrates constitute the major mass of soft electronic devices, selecting a substrate with suitable biodegradation profile will impact the overall device degradation [4]. Stretchability is an important parameter for substrates that is receiving rising attention for skin-like and biocompatible devices. Agarose and chitosan are natural biodegradable polymers with potential as substrate films for soft electronics. Plasticizers such as glycerol can enhance the functional properties of these biopolymer films by imparting stretchability and flexibility [5]. Consequently, plasticized agarose and chitosan films and their biocomposites have immense potential in replacing the existing synthetic, non-biodegradable fossil fuel-based films.

Results: Agarose, chitosan and their biocomposite films were prepared by solution casting method using glycerol as the plasticizer. The mechanical properties of these films were investigated for different ratios of biopolymers and glycerol. With increase in glycerol content, the maximum tensile stress for the agarose/glycerol, chitosan/glycerol and agarose/chitosan/glycerol films was observed to be less than 1000 kPa and the elongation at break was recorded to be more than 70%. The thermal stability of the films was also investigated using thermogravimetric analysis, which demonstrated that agarose/glycerol and agarose/chitosan/glycerol films remain stable at elevated temperatures. Additionally, the swelling and the weight loss due to leaching in water were also studied to characterize the films.

Conclusions: In this work, plasticization of agarose and chitosan biopolymers were demonstrated as means to reduce stiffness and impart stretchability in the films. The expected outcome of this work is technologies for producing soft, stretchable, and biodegradable substrate films for soft electronics that can transform into industrial scale manufacturing in future. Incorporating plasticized biopolymers and their composites into wearable and implantable electronics is expected to promote the seamless synchronization of electronics and humans.

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New Principles of Active Particle Propulsion Driven by Electrical and Chemical Gradients

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Background: Active particles can “self-propel” on the microscale, by drawing energy from their environment to power their motion. These particles offer innovative solutions to many current challenges in the biomedical field, such as targeted drug delivery and selective micro-scale surgeries, as well as environmental remediation and nanofabrication. Their main feature enabling self-motion is the principle of breaking symmetry to create a localized gradient, which can be physical or chemical. A variety of methods to induce this self-propulsion have been explored, including stimulation by magnetic,^[1,2] electric^[3], acoustic, optical, biological, and chemical^[4] means. Despite these strides, the field of active particles faces the ongoing challenge of developing new principles and functionalities. Here we present two new concepts: (1) asymmetric alternating current (AC) field propulsion that would grant multiple new degrees of freedom and (2) creating novel osmotically-driven ultra-simple superdiffusive paste made from salt particles.

Results: First, we present the findings for an asymmetric AC field-driven active system by characterizing particle velocity as a function of frequency, voltage, and size. Through our results, we reveal a new AC electrohydrodynamic effect in which spatially homogenous, temporally non-uniform signals drive colinear particle motion with respect to the electric field. By modifying the asymmetry of the AC signal, latex particles can multimodally change their direction of motion on demand. In the second project, we reveal a superdiffusive paste that demonstrates collective dispersal of rapidly dissolving particles. We found that the radial dispersion is driven by osmotic propulsion, driven by the solute concentration gradients formed by the dissolution of salt particles. We present an analysis of the critical parameters governing the system and preliminary results on the loading, rapid dispersion, and visualization of a disinfecting agent. Upon application of both “passive” and “active” disinfecting pastes to a model dermal wound from porcine gelatin, we observed a significant difference in coverage, with our active paste reaching a greater area.

Conclusions: Both of these complementary projects could have transformative impact on the field of active particles by answering fundamental questions on the role of AC-EHD effects, collective gradient-driven phenomena, and the rational design of active particle systems. Our fundamental work on the superdiffusive paste has potential to be transplanted to novel biomedical disinfection products for efficient in-vivo treatment of dermal wounds and lesions. Through interdisciplinary research, we aim to expand the knowledge boundaries in this rapidly developing research field.

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Colloidal Design of Novel Self-propelling Active Cleaners for Efficient Microplastics Remediation

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Background: With the persistence and toxicity of microplastics dispersed throughout numerous aquatic systems, microplastic removal has received attention as one of the most urgent environmental remediation problems. Conventional water treatment methods such as filtration and centrifugation are impractical for the cleaning up of such enormous volumes of natural water because of their high cost, low throughput, and disruption to aquatic life.

Results: We propose a new remediation technique based on active microcleaners. These microcleaners remove microplastic particles in the aquatic system by spreading through active motion and having hierarchical morphology enabling highly efficient capture. The active cleaners are composed of dehydrated and concentrated soft dendritic colloids (SDC). The SDCs are a new class of soft matter introduced recently by our group [1]. Their highly branched hierarchical structure mimicking the nanofiber mats from the legs of the gecko lizards leads to strong adhesion to microplastic particles via van der Waals attraction. The microcleaner SDCs are made of chitosan, a sustainable biomaterial. The dehydrated and condensed SDCs particles are infused with a small amount of fatty acid. When the acid is released slowly, it acts as “fuel” that generates surface tension gradient which makes the microcleaners self-propel on the water surface by the Marangoni effect. The self-propulsion over long distances will enable the compacted dendrimeric particles to spread over a large area of water before re-hydrating, sinking, and capturing the microparticles. This could dramatically enhance their water remediation efficiency. We first characterized how the microcleaner propulsion is influenced by the composition of fatty acid “fuel”, its surface tension and solubility, and traversed area. The active cleaners can propel for >400 s at distances >8 m at the water-air interface driven by just 0.1 μl of eugenol at a speed of > 300 mm/s.

Conclusions: We have revealed the origins of the rapid propulsion of active cleaners and established means to control and enhance it. The propulsion results in fluid shear during re-hydration, restoring the pristine SDC structure of highly branched dendrimer after propulsion. The resulting broadly dispersed rehydrated dendritic colloid can perform highly efficient microplastics capture and has considerable promise for cleanup applications in diverse aquifer types including saline seawater conditions. We believe that this research could open a new avenue for microplastic remediation in real aquatic system that is cost-effective, biocompatible, and requires less energy.

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Accelerated Synthesis of Indium Phosphide Quantum Dots in Modular Microfluidic Reactors

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Background: Continuous microfluidic flow reactors have driven the transformation of high-performing semiconductor nanocrystal synthesis into faster, cheaper, safer, and greener processes. Microfluidic platforms offer a multitude of advantages compared to conventional batch reactors, including significant reduction in chemical, high surface-to-volume ratios, and enhanced/tunable mass- and heat-transfer rates [1]. Recent efforts in Quantum Dot (QD) synthesis has been focused on the development of heavy metal-free QDs. Indium Phosphide (InP) QDs offer the same unique and highly tunable optical and electronic properties of heavy metal-based QDs without toxicological concerns for humans and the environment [2]. Despite the unique advantages of flow synthesis strategies for the controlled synthesis of InP QDs, there is still a gap between the quality of best performing reaction conditions in batch reactors and its adaptability to a continuous flow synthesis [3]. In response, we present a modular tube-based flow reactor platform for intensified multi-step synthesis of high quality InP QDs.

Results: High quality continuous synthesis of InP QDs was achieved. The quality of the as-synthesized particles was monitored in real-time via the first excitonic peak to valley ratio (P/V) of the UV-Vis absorption spectra. The highest reported P/V, 1.36, for continuous flow systems was accomplished while reducing the reaction time up to an order of magnitude than previously reported batch protocols. The first absorption peak was 490nm and was obtained using a reactor configuration that consisted of two plate-based reactors and one helical-based reactor. Increasing the total residence time in the flow reactor resulted in red-shift in the first excitonic peak wavelength and therefore the size of the in-flow synthesized QDs.

Conclusions: The modular flow chemistry strategy presented in this work presents an attractive route for accelerated development of nontoxic InP QDs. The accessible process parameters can be readily explored by the facile assembly of a library of modular flow reactors. This massive universe of potential experiments can be studied by the resulting time- and temperature-to-distance transformation of each module introduced to the overall system. The highest reported P/V, 1.36, for continuous flow systems was achieved with a first absorption peak of 490 nm. Further technological integrations such as automation and machine assisted decision making could accelerate the discovery, development, and manufacturing of higher quality colloidal nanocrystals for energy, display and chemical technologies.

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Large Amplitude Oscillatory Shear to Quantify Carbon Nanotube Composites

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Background: Roll coating is used to distribute liquid coatings onto surfaces. By tuning the rheology of the coating fluid, regular microstructures can be formed and manipulated through a phenomenon called viscous fingering. We utilize a polydimethylsiloxane-based system compounded with multi-walled carbon nanotube (MWCNT). By modulating parameters such as viscosity, relaxation time, and yield stress, the size and shape of the microstructures can be tailored and maintained to be cured into permanent structures [1]. By using oscillatory and creep rheology, the yield stress can be confirmed in two distinct ways [2]. Large amplitude oscillatory shear (LAOS) rheology, in conjunction with Fourier transform analysis, can expose large strain behavior, like strain hardening/softening and shear thickening/thinning, that first harmonic rheological characterization would not indicate [3]. Carbon nanotube composites are well studied in literature, with storage modulus increasing with increased loading and decreasing yield stress behavior with improved mixing, due to breakup of CNT aggregates [4], [5]. LAOS studies of CNT composites are limited, with one paper indicating shear thickening and strain hardening behavior for a CNT-poly(vinylidene fluoride) composites [6].

Results: To estimate the yield stress, we employed two approaches, elastic stress and creep method. Both methods show good agreement. At low CNT loadings, the yield stress of PDMS 186 composites deviate from that of PDMS 184. With increased oscillatory strain, structure shifts from elastic to viscous behavior, where with increased frequency, the system becomes more elastic, as shown via Lissajous plots. Despite having different dispersion media, the composites all have similar third harmonic phase angles, all of which are greater than 100 degrees. The pure polymers have third harmonic phase angles less than 100. For both PDMS types, the composites indicate strain stiffening and shear thinning behavior.

Conclusions: Strain hardening behavior, as indicated by LAOS measurements, corresponds well with observations in the roll coating process, as we see filament formation, which indicates a material resisting rupture. This behavior is not seen in elastic (G') and viscous (G'') behavior, as it does not show higher harmonic behavior, which has increasing contribution to the stress, as seen in the relative harmonic intensities with respect to strain.

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Background: Gelatin-based hydrogels (GHs) have been used for drug release due to their biocompatibility, tunable mechanical strength, and absorbent characteristics [1]. These properties originate from the hydrophilic net-like structure, featuring chemically crosslinked networks that expand in the presence of water, increasing the mesh size within the network and improving diffusion throughout the gel [2]. Guanidine and carboxylate moieties in GHs serve as metal ligation sites during Atom Transfer Radical Polymerization (ATRP) [3]. ATRP reactions require the presence of a rapidly activated and deactivated metal-ligand catalyst to sustain radical concentrations necessary for polymerization. These normally copper-containing catalysts prove challenging to remove from the desired polymer product, thus spurring much research into minimizing metal-ligand use and extraction methods. Here we propose using GHs to absorb and deposit ATRP precursor solutions and serve as a ligation center and reductant to replace externally added ligands and minimize the addition of copper.

Results: We investigate the (1) ability of GHs to absorb monomer precursor ATRP solution, (2) to serve as viable ligation centers for metal-ligand catalysts, and (3) confirm their role as a potential reductant of Cu(II) to Cu(I). GHs swell exceptionally well in ATRP precursor solutions for N-Isopropylacrylamide and 2-(dimethylamino)ethyl methacrylate. In the absence of externally added ligand 2,2-Bipyridine, ellipsometry revealed that GHs could conduct surface-initiated ATRP with polymer brush lengths upwards of 40 nm. Additionally, when absorbing GHs in monomer precursor solutions containing Cu(II) exclusively and depositing said hydrogels onto activated silica wafers, ellipsometry revealed polymer brush synthesis with a length of 10.7 nm. UV-Vis analysis further supported hydrogel's role in reducing Cu(II) to Cu(I) based on shifting spectral intensities from 740 nm to 430 nm.

Conclusions: We found GHs serve as a suitable candidate for (1) the absorption of surface-initiated ATRP precursor solutions, (2) ligation centers for activated Cu(I) catalysts for surface-initiated ATRP, and (3) a viable reducing agent for the activation of Cu-ligand catalysts. These findings pave the way for alternative methods of conducting ATRP reactions with minimal concentrations of added copper and ligands, eliminating costly post-reaction separations.

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Sustainable agrochemical sprays

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Background: Increased awareness of the long-term impacts of agrochemicals has resulted in the hunt for efficient and sustainable delivery platforms. In order to meet the food demands of an exponentially increasing global population, there is a dire need to establish sustainable technologies for targeted and slow release of agrochemicals with minimal environmental footprints. Furthermore, rising concerns of the global community about the accumulation and environmental effects of microplastics have accelerated the search for alternate delivery vehicles developed from biodegradable polymers [1, 2, 3]. We present a sustainable approach to synthesize aqueous dispersions of biodegradable cellulose derivatives *via* anti-solvent precipitation. We propose utilization of these dispersions as controlled and targeted release foliar spray formulations for a pesticide as a model active ingredient (AI). While biodegradable nature of our polymer particles and use of water as the dispersant medium justify sustainable nature of these formulations, the adaptability of the dispersions to cater to a range of crops and AI is exhibited through modulation of the particle shape and size through using three types of cellulose derivatives. Additionally, we have used Isothermal Titration Calorimetry (ITC) to investigate the nature of polymer interactions with the AI to provide a comprehensive picture of the performance and tenability of the formulations.

Results: Results of the study demonstrate the efficacy of the formulations for foliar AI applications. Enhanced adhesion of the dispersions on model leaf substrates under a simulated rain test signify the superior rainfastness of the formulation, while in-vitro fungal assays show the increased bio-availability of the AI due to loading on the cellulose derivative particles. The effect of particle size and morphology on AI bonding strength and release is corroborated through Isothermal Titration Calorimetry (ITC) analysis and release assays.

Conclusions: The simplicity and sustainability of the approach combined with the potential to significantly lower AI application rates for achieving the desired pest protection shows the promise of the technique to significantly impact global food security while mitigating environmental concerns related to pesticide overuse.

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New Tools for Capture and Removal of Microplastics in Aqueous Environments

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Background: The amount of plastic particles in the environment has increased substantially due to the exponential increase in plastic products production and their slow degradation rates [1, 2]. Current methods of capturing these microparticles are time-consuming, cost-prohibitive and have size limitations [3]. We provide an alternative solution of using soft dendritic colloids (SDCs), or dendricolloids, as novel means to remove microplastics from aqueous environments. The SDC particles have a unique polymeric morphology with a hyperbranched, nanofibrous corona and large excluded volume that aids the removal process [4]. In addition to sparse collection methods, little is known about microplastics themselves. This project also focuses on developing a novel millifluidic flow device (MFD) that will enable precise characterization and visualization of the formation of microplastics in simulated microenvironments in order to characterize their properties and on this basis help mitigate the release of these particles into the environment.

Results: With the focus on microplastic capture, different experimental conditions were chosen to observe the difference in behavior of the particles. In order to study the interfacial properties and how it plays a role in the heteroaggregation of dendricolloids and microplastics, their suspensions in aqueous solutions of different ionic strength and pH ranges were investigated. The highest capture efficiency was found around 0.1 and 0.6 M NaCl, which is approximately the salinity of the ocean. For the pH range, the highest capture efficiency was pH 7.5 and 8.5. Polystyrene microbead models of different sizes and functional groups were tested and compared as well. This enabled a deeper investigation of the role of the interfacial properties of the SDCs and microplastics found in different environments. A prototype of the MFD was made from acrylic with nylon screws for transparency and UV resistivity. MFD is currently being tested with experimental runs under UV.

Conclusions: This project will enhance the understanding of interactions between SDCs and microplastics as a function of their interfacial properties. Based on the results, we theorize that both van der Waals and electrostatics play a role in microplastic adsorption. With the help of the MFD we can gain insight how to develop highly efficient microcleaners for microplastic remediation in aqueous environments.

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Applications of Soft Dendritic Colloids in Li-ion Batteries

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Background: The Li-ion battery has dominated the energy storage industry since its commercialization in the early 1990's. The high energy density and low self-discharge rate of Li-ion cells has enabled their capture of the portable power market. However, the components within Li-ion batteries remain largely unchanged over the last 30 years. To keep up with evolving quantity and performance demands of the market, Li-ion battery technology and manufacturing techniques must evolve. A novel morphology of polymer particles known as soft dendritic colloids (SDCs) was discovered by the Velev group at North Carolina State University [1]. These high-aspect ratio particles are manufactured by a facile shear-driven solvent/non-solvent induced phase separation method. The high surface area and entanglement make these structures an ideal candidate for electrochemical systems, which rely on efficient surface phenomena. Herein we report applications of these structures in both Li-ion battery separators and electrodes.

Results: Three different morphologies of SDCs were formed by varying the concentration of the injected polymer, poly(vinylidene difluoride) (PVDF). Each of these three unique morphologies were vacuum filtered to form fibrous and highly porous battery separators. The SDC non-woven separators showed far superior electrolyte uptake and ionic conductivity compared to their commercial analogues as well as comparable cycling stability in Li-ion half cells [2,3].

SDCs were also formed out of redox active polymers (e.g. poly(2,2,6,6-tetramethyl-piperidinyloxy-4-yl methacrylate) (PTMA)) to form composite electrodes with carbon material. Optical and electron micrographs confirm the branched morphology of the electrodes. Charge-discharge and impedance experiments are carried out in Li-ion half cells with results presented in the poster.

Conclusions: This project illustrates how SDCs can be used to fabricate improved electrochemical device components, including but not limited to the electrodes and the separators. Shear-driven solvent/non-solvent induced phase separation is also demonstrated as an all-in-one manufacturing platform for Li-ion battery components.

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Smart Manufacturing of Metal Halide Perovskite Nanocrystals

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Background: Metal halide perovskite (MHP) nanocrystals (NCs) have been of great interest in optoelectronics due to their size- and composition-tunable optical properties, high photoluminescence quantum yield (PLQY), large absorption cross-section, and facile solution-phase synthesis. Despite the unique optical and optoelectronic properties of MHP NCs, their large-scale adoption by printed energy technologies are hampered by the lead toxicity and instability against light, moisture, heat, and electric field. Recently, cesium copper halide NCs with narrow size distributions and tunable emissions have emerged as a promising lead-free MHP NC candidate, with near unity PLQY. [1, 2, 3] However, the fast formation kinetics of copper-based MHP NCs resulting in batch-to-batch variation, complicates their fundamental and applied studies.

Results: Herein, we report a modular flow chemistry platform directed by machine learning (ML) to autonomously synthesize cesium copper halide perovskite NCs with the desired optical properties. Utilizing the developed flow chemistry platform, we study the effects of halide composition, precursors concentration, reaction time, and temperature on the optical properties of the as-synthesized and purified copper-based MHP NCs. Furthermore, we investigate role of metal halide additives on controlling the morphology uniformity and optical properties of the in-flow synthesized MHP NCs. Utilizing Bayesian Optimization (BO), we demonstrate the unique potential of modular flow reactors for accelerated parameter space mapping and on-demand synthesis of rapidly optimized MHP NCs with minimum experimental cost.

Conclusions: In summary, copper-based MHP NCs were autonomously synthesized in a miniaturized flow reactor equipped with an online spectral monitoring probe. The autonomous flow chemistry strategy detailed in this work enables accelerated discovery of lead-free MHP NCs while minimizing chemical consumption and waste generation. The high-performing MHP NCs synthesized in this work could pave the way for large-scale adoption of nontoxic MHP NCs by printed clean energy technologies.

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Chemically defined synthetic matrix models early interaction between fetal cytotrophoblast and uterine stromal cells

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Background: One of the first events that must occur in pregnancy is the blastocyst implantation into the maternal endometrium. Defects in implantation and placentation often result in numerous pregnancy complications. Trophoblast stem cells give rise to the other tissues of the placenta. Thus, early interaction between trophoblast and the maternal endometrium is critical for proper implantation. Ethical restrictions on research with human embryo and fetal tissues and mechanistic differences in human and animal models, molecular mechanisms underlying early human trophoblast development remain poorly understood. Our research here employs a multi-disciplinary bioengineering approach to develop a synthetic extracellular matrix (ECM) model with gelatin methacrylate (GelMA) hydrogel. Our system enables mechanistic studies on trophoblast differentiation to invasive extravillous trophoblast (EVT) in vitro in a 3D culture system. EVT cells are vital to anchor the developing placenta from fetal end into maternal decidua. Our 3D system allows us to study matrix degradation and cell migration, important process in in vivo EVT differentiation. Among the current 2D and 3D in vitro culture models to recapitulate EVT invasion in the maternal endometrium, 2D models do not provide insight into molecular mechanisms regulating EVT differentiation in vivo. Also, current 3D models widely use poorly defined Matrigel as ECM, derived from tumor tissue, and limit mechanistic studies of EVT differentiation in 3D culture.

Results: Our micro-engineered quantitative EVT invasion model can reconstruct the three-dimensional structural organization of the maternal endometrium with a chemically defined synthetic ECM. We can also study the crosstalk between endometrial stromal cells and trophoblast cells with our 3D model. Our results show the important role of decidualized stromal cells plays as a regulator of extravillous trophoblast invasion.

Conclusions: This work will help to understand the molecular mechanism behind physiological and pathological processes of trophoblast-endometrium interaction during early placenta development.

Flexible Sensor Patch for Continuous Carbon Dioxide Monitoring

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Background: Monitoring and measurement of carbon dioxide (CO₂) is critical for many fields. The gold standard CO₂ sensor, the Severinghaus electrode [1], has remained unchanged for decades. In recent years, many other CO₂ sensor formats, such as detection based upon pH-sensitive dyes, have been demonstrated, opening the door for relatively simple optical detection schemes [2], [3]. However, a majority of these optochemical sensors require complex sensor preparation steps and are difficult to control and repeatably execute. Here, we report a facile CO₂ sensor generation method that suffers from none of the typical fabrication issues [4].

Results: We utilized polydimethylsiloxane (PDMS) as the flexible sensor matrix and 1-hydroxypyrene-3,6,8-trisulfonate (HPTS), a pH sensitive dye, as the sensing material. HPTS, a base (NaOH), and glycerol are loaded as dense droplets into a thin PDMS layer which is subsequently cured around the droplet. The fabrication process does not require prior knowledge in chemistry or device fabrication and can be completed as quickly as PDMS cures (~2 h). We demonstrated the application of this thin-patch sensor for in-line CO₂ quantification in cell culture media. To this end, we optimized the sensing composition and quantified CO₂ in the range of 0-20 kPa. A standard curve was generated with high fidelity ($R^2 = 0.998$) along with an excellent analytical resolution of 0.5 kPa (3.7 mm Hg). Additionally, the sensor is fully autoclavable for applications requiring sterility and has a long working lifetime.

Conclusions: CO₂ monitoring has been a focus of analytical device development for almost 70 years. We developed what we believe is the simplest to fabricate CO₂ sensor to date that is also capable of continuous monitoring in real time and is robust enough for long term storage as well as exposure to harsh conditions such as autoclaving. This flexible, simple-to-manufacture sensor has a myriad of potential applications and represents a new, straightforward means for optical carbon dioxide measurement.

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Discovery of Peptide Inhibitors of *Clostridioides difficile* Toxin A

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Background: *Clostridioides difficile* is an opportunistic pathogen that exploits disruptions in the commensal microbiome of the gastrointestinal tract. *C. difficile* infection (CDI) is characterized by colitis and diarrhea, which are largely caused by two secreted toxins, TcdA and TcdB. These primary virulence factors glycosylate Rho-family proteins, thus disrupting Rho-dependent cellular processes and leading to inflammation and increased epithelial permeability [1]. Treatment of CDI typically involves the withdrawal of antibiotics mediating the gut dysbiosis that allows *C. difficile* to flourish, and the initiation of vancomycin, metronidazole, or fidaxomicin [2, 3]. While this is often effective, about 20% of cases develop protracted infections that may persist for multiple years [4]. Increasing prevalence of hypervirulent strains and growing antibiotic resistance are further hampering antibiotic treatments [19]. The increasing risk of CDI and shortcomings of current treatment options poses an urgent need for novel therapies.

Results: Novel peptide inhibitors of *C. difficile* TcdA were identified through experimental and computational peptide screening. Seven TcdA binding peptides identified through solid phase peptide library screening and seven putative TcdA glucosyltransferase domain (GTD) binding peptides identified from the *peptide binding design (PepBD)* were screened for potent binding to the GTD using an in-house microfluidic device and bead-based peptide display system. Eight peptides displayed promising TcdA GTD binding properties and were tested for TcdA inhibition in primary human small intestine and colon epithelial models. One peptide completely prevented the loss of transepithelial electrical resistance (TEER) associated with TcdA-mediated cytotoxicity in the primary human colon model. Another peptide partially restored TEER in the primary human colon model. The lead peptide exhibits strong binding to TcdA with a K_D of 56.1 ± 29.8 nM as measured by Surface Plasmon Resonance.

Conclusions: The combination of computational and experimental approaches allow for the rapid identification and testing of novel peptide inhibitors to gastrointestinal toxins.

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Tools & Methods for Engineering Colonization of Plant Microbiomes

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Background: Enhancing crop production is a necessity with increasing demand for staple crops and utilization of carbon/nitrogen.¹ Plant-associated microbiomes offers one avenue for addressing this demand.²⁻⁴ While large advancements have been gained recently due to advancements in high-throughput technology, building enhanced or new functionality into existing microbiomes has remained a challenge due to sparse materials and methods along with poor colonization of the desired trait.¹

Results: In the work discussed here, we detail the development of genetic tools and utilization of these tools for elucidating colonization factors into the Maize microbiome using a model synthetic community (SynCom). Utilizing this simple yet representative SynCom, we have been able to develop highly efficient and standard transformation methods of over 10^6 CFU/ug of DNA. Furthermore, we have developed standardized genetic expression and transformation vectors by utilizing these transformation protocols to rapidly characterize endogenous regulatory sequences for variable protein expression. Finally, we discuss the current work utilizing all components to identify functions that enhance SynCom member colonization of the plant host.

Conclusions: Overall, the tools and methods outlined in this work provide researchers a standardized platform to interrogate host-microbe interactions for the maize root system. We show how to utilize these tools in a high-throughput fashion to rapidly characterize regulatory sequences and elucidate sorely needed functional genes for enhancing microbiome colonization.

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Inducible Directed Evolution of an Anticancer Terpene Biosynthetic Pathway in *E.coli*

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Background: A central challenge in metabolic engineering lies in identifying the correct expression levels and activities of enzymes that lead to the production of a desired product. While a plethora of methods enable efficient exploration of expression space for entire metabolic pathways, enzymatic activity improvements are primarily achieved through directed evolution of single enzymes. We wished to understand whether directed evolution of more complete metabolic pathways would lead to greater productivities than evolution of single enzymes alone. To do this, we took production of (S)-(-)-perillyl alcohol (POH), a putative anticancer molecule, as a case study [1]. Studies have shown that POH and its derivatives can pass the blood-brain barrier and treat glioblastoma with few side effects. The low amounts that can be isolated from plant sources, as well as the complexity and high cost of chemical synthesis, has made microbial production an ideal platform for POH synthesis. We have developed a minimal, highly efficient enzymatic pathway for POH biosynthesis in *E. coli* and a transcription factor-based biosensor to detect POH production *in situ* [2]. However, further improvement in productivity has been hampered by the difficulty of evolving the large POH biosynthetic pathway (~ 10 kb).

Results: To solve this issue, we used Inducible Directed Evolution (IDE), which is capable of evolving DNA sequences up to 36 kb in length. Specifically, we used a mutagenesis plasmid to introduce random mutations into the POH biosynthetic pathway, followed by transfer into a biosensor-containing strain via a temperate bacteriophage. Variants with high cellular fluorescence, corresponding to high POH productivity, were recovered by multiple rounds of fluorescence-activated cell sorting spanning over 10^6 variants, and the spectrum of mutations present during each round were determined by sequencing.

Conclusions: These results demonstrate the utility of inducible directed evolution for biosensor-enabled screens and point to a pathway-wide framework for performing directed evolution on multigene metabolic pathways.

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Engineering Vibrio natriegens for Upcycling Poly(ethylene terephthalate)

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Background: Poly(ethylene terephthalate) (PET) has become a major global concern due to its accumulation and resistance to degradation in the natural environment. Current strategies for recycling waste PET have been applied to alleviate PET pollution. However, some recycling processes can cause secondary pollution by consuming massive amounts of energy and utilizing hazardous solvents. Moreover, the amount of recycled PET is limited and much less than the amount of PET that ends up in the landfill. Consequently, the majority of PET waste is further broken down into microplastics whose dimension smaller than 5 mm. The leakage of microplastics into the ocean can threaten marine lives and ecosystems, and further jeopardize human health through the food web. Our project focuses on developing a remedy for PET microplastics by applying metabolic engineering to construct a whole-cell biocatalyst for degrading and assimilating waste PET in situ. *Vibrio natriegens*, a fast-growing, nonpathogenic, salt-tolerant marine bacteria, is the ideal chassis to achieve this bioremediation purpose.

Results: Firstly, we engineered *V. natriegens* to express PET-degrading enzymes. A two-enzyme system composed of PETase and MHETase was discovered in *Ideonella sakaiensis* and was demonstrated to degrade PET efficiently at ambient temperature [1]. We fused these two enzymes to a surface anchor, successfully constructing a *V. natriegens* that displays enzymes on its outer membrane. We verified the surface display by using immunocytochemistry and demonstrated the function of enzymes by using liquid chromatography to analyze the enzymatic reaction products. After hydrolysis by PETase and MHETase, PET is broken down into terephthalic acid (TPA) and ethylene glycol (EG). Therefore, we constructed a metabolic pathway for assimilating TPA in *V. natriegens*. TPA is commonly metabolized via enzymes that convert TPA into protocatechuic acid (PCA), followed by further catabolism through the benzoate pathway. Since *V. natriegens* can grow in minimal media with PCA as the sole carbon source, we further enabled TPA catabolism in *V. natriegens* by expressing the necessary transporters and metabolic enzymes, then demonstrated its growth using TPA as a sole carbon source for the first time. Finally, we will couple the PET depolymerization and TPA degradation and provide an efficient platform for applying directed evolution to expedite PET degradation.

Conclusions: Our project proposes a sustainable *in situ* bioremediation strategy for PET microplastic pollution. The engineered *V. natriegens* with the two-enzyme system may be able to perform as a whole-cell catalyst that can be easily separated or recycled by centrifugation and proliferated by cultivation so that it can overcome the major limitation of enzymatic PET recycling-product inhibition. Our research also contributes to the advancement of synthetic biology by expanding the genetic toolkit of *V. natriegens*, an under-characterized bacterium with superior growth rates. Taken together, this work expands the knowledge about engineering *V. natriegens*, and establishes a promising strategy for mitigating PET accumulation in seawater.

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In vitro human platform to efficiently study Angelman Syndrome Class I/II deletion genes

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Background: Angelman Syndrome (AS) is a neurodevelopmental disorder characterized by mental disability, speech impairment and ataxia. Deletions and loss-of-function mutations at chromosome 15q11-13 locus can lead to AS [1]. The most common etiology of AS is Class I/II deletions which comprises about 70% of the cases. These large deletions span at least 5 million base pairs on chromosome 15 leading to loss of many genes including *UBE3A* [2-4]. *UBE3A* has been reported to be responsible for the core symptoms of AS [5] and hence has been the focus of AS research. However, AS individuals with large chromosome deletions show more severe symptoms [4, 5] indicating that *UBE3A* and its surrounding genes collectively contribute to the disease pathology of AS. Therefore, we need human-specific platforms that will enable us to study *UBE3A* and its understudied neighboring genes.

Results: We are working on establishing an isogenic AS platform which will enable us to study Class I/II deletion genes. Accordingly, we are pursuing two approaches in parallel: (i) Designing and integrating a recombinase-based landing pad into a safe harbor locus of AS-patient derived cell lines to rescue the expression of Class I/II deletion genes, (ii) Generating AS Class I deletion cell lines from human embryonic stem cells. We successfully designed a landing pad and integrated it into the AAVS1 safe harbor locus of H1, H9 and AS Class I deletion cell lines. We are in the process of testing the recombination efficiency of the landing pad-integrated AS Class I deletion cell line. Once this is validated, we will start rescuing the AS Class I/II deletion genes. In parallel, we are using CRISPR/Cas9 to induce large deletions in H1 and H9 cells to create isogenic AS Class I/II deletion cell lines.

Conclusions: The aim of this study is to construct an AS platform derived from human pluripotent stem cells which will help us investigate the genes that are lost in AS Class I/II deletion. This platform will be isogenic and human-specific; hence it will serve as a good disease model for AS.

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Neuronal Injury patterns of highly branched dendrites in *C. elegans* neurons.

Kin Gomez[1], Adriana San-Miguel[1]

1. Dept. of Chemical and Biomolecular Engineering, NCSU

Background: Many of the biochemical and metabolic pathways that are present in *C. elegans* have analogues to the human system; this makes it a good model to test questions regarding neuronal injury^[1]. The PVD neuron pair is a well-studied highly branched neuron that is responsible for the sensation of touch, and cold, detection of sound, and proprioception in *C. elegans*. This neuron type develops age-related beads that are associated with the action of autophagosomes as seen in mammals^[2]. In a previous study in our lab, it was identified that exposure to cold shock can also induce beading in PVD. Beads induced by cold showed a different spatial arrangement than those caused by aging^[3]. It is unclear if all beading depends on the same mechanisms or if there are multiple biochemical pathways that result in the formation of blebs of similar visual characteristics^[2,4,5]. Previous studies suggest a relationship between beads presence and the functionality of the neuron^[2,6].

Results: The Glutamatergic neuron PVD showed susceptibility to exposure to hypoxic stress. After reducing the oxygen atmosphere to about 7%, the population showed a significant increase in visible dendritic beading. After exposing the worms to a full anaerobic condition, no injury was observed. In contrast to the beading induced by cold exposure, hypoxic beading is not reversible. Together these results suggest that the induction of injury derived from anoxic stress requires metabolic activity and acts through a different pathway than cold-induced beading. When performing experiments in liquid, control populations showed high variability in their neuronal structure integrity. The mechanism that generates this stochastic behavior is an open question that could lead to a different injury mechanism.

Conclusions: The induction of neuronal through different insults results in specific characteristics like the intensity of the injury and reversibility. As shown before^[4], by using neuronal networks it would be possible to elucidate spatial differences that are also present in the populations injured through different means. The next steps for this project will be to analyze the data sets with computational tools and then use the results to determine the molecular and genetic mechanisms involved in each stress scenario.

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Extreme thermophily resists contamination and offers unique product separation opportunities for plant biomass fermentations

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Background: Microbial degradation and conversion of plant biomass into industrial products has been investigated as an alternative to fossil-derived chemicals. Consolidated bioprocessing aims to deconstruct and convert plant biomass in a single step. Certain extremely and moderately thermophilic bacteria (Such as *Caldicellulosiruptor bescii* and *Acetivibrio thermocellus*) stand out as major candidates due to their native ability to deconstruct complex (hemi)cellulolytic substrates without pretreatments [1]. Production of valuable products in these microbes at industrially relevant levels still remains a barrier to commercial use, although production of several commercial chemicals has been demonstrated, including acetone, butanol, and ethanol [1,2,3].

Results: Extreme thermophily offers significant advantages compared to mesophilic and moderately thermophilic counterparts, allowing for novel product separation strategies and increased resistance to contamination. Here, we will present work that investigates and exploits these advantages. We will present further progress in engineering *C. bescii* to produce volatile chemicals (acetone, ethanol) at extreme temperatures ($>70^{\circ}\text{C}$) to enable *in situ* separation of desired products from fermentation headspace (dubbed ‘bioreactive distillation’), including an in-depth process model and techno-economic analysis [4]. We also investigate and define a thermophilic threshold for plant biomass fermentations, where operation above this threshold resists contamination from microorganisms indigenous to plant biomasses.

Conclusions: Techno-economic analysis indicates the feasibility of extreme thermophiles for industrial fermentations, and highlights unique capabilities of *C. bescii* to degrade plant biomass feedstocks (soybean hulls, transgenic poplar). This work defines specific metabolic engineering targets for on-going work to produce acetone with *C. bescii*. Additionally, work to understand contamination risks in plant biomass fermentation defined a thermophilic threshold to resist contamination as 75°C ; thus extreme thermophily is adventitious as it offers potential to reduce costs associated with sterilizing pretreatments for industrial biomass fermentations.

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Characterization of Solid-State DNA Transfer for DNA-based Data Storage

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Albert Keung [1], James Tuck [2]

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Background: Digital information is omnipresent in our lives, from emails to social media to medical records. In 2020, the total amount of data created was 64 zettabytes (ZB), and it is projected to increase to 175 ZB by 2025. This capacity correlates to ten trillion downloads of an HD *Forrest Gump* movie. Most archival data are stored in massive data centers, but the global demand and growth of data are quickly surpassing the synthesis of archival storage media like tape drives. DNA can be used as an alternative storage medium as it is more durable, compact, and capable of denser storage. In fact, its storage capacity is at least a million times denser than a tape drive. To utilize this system, data is encoded into nucleotide sequences that are synthesized to form the database. Pre-existing synthesis methods use liquid handling of phosphoramidite or molecular biology reagents, which use similar technologies to inkjet printing. However, these approaches result in high solvent volumes and limitations on synthesis speeds due to mechanical components. In comparison, laser printers use toner powder to print, resulting in a larger density of “ink” at a lower volume. In addition, they can print 10 times faster than inkjet printers. Laser printers use electrostatic interactions to move the toner powder to the selected areas and fuse it to the paper by melting it. Here, we use the same technology to explore the direct electrostatic transfer of solid-state DNA.

Results: Previously, we have shown that we can laser-print DNA using black toner. We were then able to extract the DNA from the printed area and quantify it. Now, we are expanding our findings to assemble DNA-based files using this technology. We started with a plate model to simulate the laser printer set-up. The plate model was used to determine a quantifiable and optimal amount of DNA to use while minimizing reagent costs. We used the QuBit Fluorometer and a propidium iodide fluorescence assay to quantify the transferred DNA with high sensitivity. Here, we transferred DNA from one stock well to multiple wells, so the stock plate was used to assemble many iterations of sequences. We plan to expand DNA synthesis and assembly with our system through ligation and PCR reactions, therefore, we needed to characterize the effects of black toner on these reactions. So, we mixed DNA with black toner to determine the tolerance limit before the enzymatic efficiency is impaired. The PCR and ligation reactions are unaffected by black toner up to a concentration of 16.25 g/L.

Conclusions: Solid-state DNA can be precisely transferred and used in enzymatic reactions for DNA-based data storage. This technology enables easier transportation of DNA and can be expanded for use in biosensors or vaccines where space and power are scarce.

Information storage via immobilization of encoded DNA on ultra-high surface-area magnetic soft dendritic colloids

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Background: DNA could enable a colossal technological leap for future digital data storage due to its high storage density, longevity [1], and energy efficiency [2]. A generic DNA-based information storage system includes database synthesizing, information accessing and reading. While previous research has focused on improving the efficiency of database synthesis and information reading, a key challenge remained as how to efficiently access a specific set of information from a large complex system. One must find solutions to how file-encoded DNA strands are copied, separated, and purified in the batch processes. Here, we propose to immobilize the DNA database on a very high surface area, high accessibility, 3-dimensional soft dendritic scaffold in a continuous packed-bed reactor. The new design would allow information to be copied and accessed by flowing reagents through the immobilized file-encoded strands.

Results: Soft dendritic colloids (SDCs) are formed through precipitating dissolved polymer in a turbulent flow of nonsolvent. Shear stress from the turbulence pull the precipitated microdroplets into a highly branched morphology with ultra-high surface area [3]. Magnetic nanoparticles are added to the dissolved polymer solution to make magnetic-responsive SDCs, which allows their remote manipulation and easy separation of SDCs from the liquid. Multiple chemical washes are performed to alter the surface of SDCs into binding sites for DNA strands. We observe both physical and chemical binding between SDCs and DNA strands. To quantify bound DNA strands, we use reverse transcription followed by real-time polymerase chain reaction.

Conclusions: In this research, we aimed to understand and control the efficiency of binding the file-encode DNA to the soft dendritic colloids (SDCs). This can be achieved by 1) incorporating magnetic nanoparticles into SDCs, 2) separating colloidal particles using a generic magnetic stand and 3) dispersing the SDCs in aqueous solutions and activating their surface with chemicals to allow binding of fluorescently labeled DNA. This work lays the foundation of developing a colloidal DNA-based storage system which has the potential to provide a cost-effective, energy-efficient, and long-lasting alternative at a time of rising concerns in global digital information storage.

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Life in Hot Acid: Exploring Key Mechanisms for Chemolithoautotrophy in Thermoacidophiles Through Comparative Phenotyping and Genotyping

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Background: The archaeal order Sulfolobales which thrive in hot acid environments ($T_{\text{opt}} \geq 65^{\circ}\text{C}$, $\text{pH} < 4$) and leverages a diverse set of metabolic pathways to survive in these conditions^[1]. Of particular interest are the mechanisms by which these organisms conserve energy from inorganic sources such as sulfur and iron to power CO_2 fixation. These mechanisms have garnered interest in biomining, due to their ability to solubilize ore-bound metal in the process of metabolizing these inorganic energy sources. In addition, using non-carbon energy sources to drive CO_2 fixation presents an opportunity for biosynthesis of industrial organic compounds directly from CO_2 ^[1]. One member of the Sulfolobales is *Sulfolobus acidocaldarius* (*Saci*), an obligate heterotroph^[2] and one of the few Sulfolobales with tractable genetic tools for metabolic engineering^[3]. In order to engineer *Saci* for biomining or chemolithoautotrophic chemical production, a deep understanding of the mechanisms for these phenomena is necessary to identify the key components of sulfur/iron oxidation, energy conservation, and CO_2 fixation. Recently, published genomes of numerous Sulfolobales species has enabled the connection of phenotype and genotype to identify these components^[4-5].

Results: Phenotypic evaluations of Sulfolobales species with regards to sulfur/iron oxidation and bioleaching were used to categorize the Sulfolobales by their ability to perform these functions. A pangenome database for the Sulfolobales was generated to identify orthologous protein clusters in the order, which underwent annotation to predict functionality of these clusters. A phenotype clustering score was applied to identify key proteins related to sulfur/iron oxidation and bioleaching. Coupled with thermodynamic analysis of abiotic sulfur chemistry^[6], this analysis identified target genes for sulfur oxidation which were engineered into *Saci*.

Conclusions: Combined phenotype and genotype comparisons identified several key genes related to sulfur oxidation and energy conservation. When combined with the thermodynamic analysis of sulfur chemistry, this analysis implicates a tetrathionate hydrolase as an essential enzyme for sulfur oxidation. The engineered strain of *Saci* demonstrated improvements in sulfur oxidation and energy conservation as a result of the additional target genes. However, further efforts are needed to reach the level of native sulfur oxidation.

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4. Counts, J.A., D.J. Willard, and R.M. Kelly (2021). *Environ. Microbiol.* **23**, 3568-3584.
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Biomining of Critical Metals Using Engineered Thermoacidophiles

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Background: One of the main disadvantages of traditional methods of metal mining is the environmental impacts including the resulting wastewater containing toxic chemicals. Novel technologies are needed to decrease environmental side effects of metal extraction from ores. Bio-hydrometallurgical methods have shown promising potential to do so. In this case, bioleaching, the process of extracting metals using microorganisms, has been explored as one of the better alternatives to traditional metal ore extractions. Specifically, for copper bearing ores, such as pyrite and chalcopyrite, successful iron and copper extraction has been reported. Application of thermoacidophiles have been explored recently, these can survive in high temperatures, which would alleviate passivation, as well as evolving in acidic environments, which would enhance metal solubility. One of the ways of improving bioleaching would be by developing engineered bioleaching strains to overcome the limits in the wild type counterparts. Ideally, the organism should be able to oxidize iron for better metal extraction, as well as sulfur to reduce passivation. In this study, thermoacidophiles with different range of iron and sulfur oxidizing capabilities are studied for pyrite and chalcopyrite bioleaching to elucidate the underlying mechanisms of thermophilic bioleaching. In addition, transcriptomic studies will be used to identify the key genes involved in bioleaching and their functions.

Results: The results have indicated that total iron extraction from pyrite can be carried out using thermoacidophiles. However, the comparison of sulfur oxidizers and iron oxidizers have revealed that sulfur oxidation is more critical for higher final metal extractions. Whereas, iron oxidizing thermoacidophiles have higher rates of bioleaching, which is done by regeneration of ferric iron for mineral oxidation, but the final metal solubilization is lower than the sulfur oxidizer. X-ray photoelectron spectroscopy studies on cultures containing high ferrous iron content with iron oxidizing strains have revealed that excess iron in the media leads to formation of iron-sulfur compounds leading to solid precipitation, which was also observed in pyrite bioleaching. Therefore, while ferrous iron oxidation to ferric iron is needed for higher bioleaching rates, sulfur oxidation is needed to mitigate passivation effects to reach high metal recovery targets. A cluster of genes, named the *fox* cluster, are known to be vital to iron biooxidation. FoxCD takes the electrons from Fe(II), which are shuttled either through the downhill (FoxA1, FoxA2, and FoxB) or the uphill electron transport chain (FoxG and FoxCD) [1]. The exact roles of other components are still in question.

Conclusions: Bioleaching of metal sulfide minerals, such as pyrite and chalcopyrite, is a complex phenomenon involving a variety of chemical reactions, biological effects, and surface interactions. Incorporation of several characterization techniques and different bioleaching strains are needed to reveal the mechanisms involved. Furthermore, iron and sulfur oxidation by the microorganisms affect the bioleaching outcome, making the study of the biological pathways involved necessary.

References:

1. Wheaton, G. et al. 2015. The confluence of heavy metal biooxidation and heavy metal resistance: implications for bioleaching by extreme thermoacidophiles. *Minerals*. 5, 3 (2015), 397–451.

Deriving PLC γ Single-Molecule Activation Statistics from Deterministic Simulations

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Background: Phospholipase C- γ (PLC γ) is a receptor-activated enzyme and plays a critical role in signal transduction, notably in the contexts of fibroblast directed motility and T-cell activation. Kinetic models [1], based on structural data [2], have offered insight into the receptor-mediated regulation of PLC γ , highlighting the importance of the interplay between tyrosine 783 phosphorylation, a hallmark of activation, and the strength of enzymatic autoinhibition. Building on this structure-based model, we devised a scheme for deriving expected dwell-time and activation statistics from deterministic solutions to the system of ordinary differential equations (ODEs). Importantly, these expected statistics can be directly compared to *in vitro* single-molecule activation experiments performed on supported lipid bilayers

Results: We confirmed that the probability density functions derived from the ODE simulations aligned with histograms generated from single-molecule stochastic simulations. We found that hypothetical mutations that alter either autoinhibition or membrane affinity can be distinguished based on their effects on rejection time, activation time, and post-activation dwell-time distributions

Conclusions: We identify a methodology to derive expected membrane association/dissociation statistics based on a structure-based kinetic model of PLC γ activation. Pairing these expected statistics with *in vitro* single-molecule activation experiments will offer mechanistic insight into how cancer-associated mutations enhance PLC γ activity. Additionally, this framework for linking structure-based kinetic models to *in vitro* experiments can be adapted to investigate the activation kinetics of other autoinhibited enzymes.

References:

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2. Hajicek N, Keith NC, Siraliev-Perez E, Temple BR, Huang W, Zhang Q, Harden TK, Sondek J. Structural basis for the activation of PLC- γ isozymes by phosphorylation and cancer-associated mutations. *Elife.* 2019 Dec 31;8:e51700

Student Resume Packet

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EDUCATION

North Carolina State University, Raleigh, North Carolina

May 2024 (expected)

Master of Science (M.S.), Chemical and Biomolecular Engineering | Current GPA: -/4.00

Relevant coursework: Polymer Science and Technology, Chemical Engineering Process Modelling and Chemical Reaction Engineering

Anna University, Chennai, India

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Bachelor of Technology (B.Tech.), Chemical Engineering | GPA: 8.66/10.00 (First Class Honnors)

RESEARCH EXPERIENCE

Anna University

Multi-Orifice Oscillatory Baffled Column

Oct 2017 – May 2018

Research Advisor: Dr. Kannan

- Designed and fabricated a new column for the treatment of hazardous wastewater and various applications.
- Studying the reaction kinetics and hydrodynamics bubble distribution behavior in the MOBC Reactor.
- Treating the tannery effluent and other Industrial effluent via Advanced Oxidation Process.
- Study had been carried out on both batch & continuous flow basis and understand the variations in efficacy of treatment.

Multi-Orifice Multi-Impeller Baffled Column

Jun 2017 – Sep 2017

- Comparative study was carried out on treating of tannery effluent with various disinfectants.
- The model has a drastic control over parameters of hazardous content and recovered metals like Ni and Cr.
- Increased the intensity of mixing of the reactor by modifying the equipment and also it was benchmarked against Gas-Sparged Stirred tank reactor.

Aerosolization Burner

Jun 2016 – Mar 2017

- Designed and fabricated a new model of burner, especially suitable for wax as a fuel.
- Increased calorific value of the burner by optimizing the flow rate of wax and water.
- Compared the efficiency of the burner with currently used heating elements (Coil, LPG, and Induction).

PROFESSIONAL EXPERIENCE

Trainee Engineer, Arabian Pipeline & Services Co. Ltd (ANABEEB), Saudi Arabia

Aug 2019 – July 2020

- Improving the commissioning techniques by exploratory research.
- Attending the seminars with clients to refine the commissioning procedures and technical supports.
- Trouble shooting the difficulties arises in the pre-commissioning works of process equipment and pipelines.

Production Engineer (Jr.), Smart Cool Systems, India

Sep 2018 – July 2019

- Analyzing the equipment layout, workflow, assembly methods, and manpower utilization.
- Confer with vendors in determining product specifications of refrigeration equipments and evaluate products according to quality standards and specifications.
- Support company policies and procedures, goals and objectives, and good manufacturing practices.

TECHNICAL SKILLS

- UV-Spectrophotometer for analyzing metal ions.
- HPLC Chromatography to identify different solutes of complex mixture.
- Proficient in using MS Office, C++, MATLAB, and ASPEN PLUS V8.0.

Fazel Bateni (Greencard holder)

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EDUCATION

Ph.D., Chemical Engineering

North Carolina State University, Raleigh, North Carolina, USA

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GPA:3.94/4.0

M.Sc., Chemical Engineering

Ohio University, Athens, Ohio, USA

August 2017-July 2019

GPA:3.86/4.0

M.Sc., Chemical Engineering

Amirkabir University of Technology, Tehran, Iran

August 2016-June 2017

GPA:17.84/20.00

B.Sc., Chemical Engineering

Amirkabir University of Technology, Tehran, Iran

August 2012-May 2016

GPA:18.29/20.00

INTERNSHIP

Scientist intern at GlaxoSmithKline (GSK)

Vaccine Research and Development Center, Rockville, Maryland, USA

June 2022-

August 2022

- Continuous manufacturing of m-RNA lipid nanoparticles vaccines for COVID-19
- Process analysis technology (PAT) development for in-line characterization via near IR spectroscopy

PROFESSIONAL EXPERIENCE

Graduate Research Assistant, Department of Chemical and Biomolecular Engineering, North Carolina State University, 2019-Present

- Developed novel flow chemistry platforms for (i) post-synthetic room-temperature and (ii) high-temperature metal cation doping of colloidal quantum dots.
- Developed a computer-controlled modular microfluidic platform for on-demand continuous manufacturing of semiconducting colloidal nanomaterials.
- Unveiled and proposed fundamental mechanisms of metal cation doping of colloidal quantum dots.
- Developed and integrated self-optimized artificial intelligence-guided decision-making algorithms to the microfluidic platform for intelligent manufacturing of metal cation-doped quantum dots.

Graduate Research Assistant, Department of Chemical and Biomolecular Engineering, Ohio University, 2017-2019

- Developed non-noble metal and metal oxide electrocatalysts for electrochemical conversion of lignin.
- Characterized morphology, crystalline structure and surface area of the electrocatalysts.
- Optimized activity, selectivity and durability of the electrocatalysts for selective production of aromatic compounds and simultaneous evolution of hydrogen in an alkaline lignin electrolysis cell.

- Constructed alkaline-based anion exchange membrane electrolyzer setup for upgrading lignin-derived compounds.
- Investigated and optimized the effects of operating conditions, including catalyst loading, initial concentration of lignin and residence time on yield of low molecular weight aromatic (LMWA) products.

TECHNICAL SKILLS

Materials	UV-Vis and PL spectroscopy, GC-MS, TEM, SEM, BET, XRD, FTIR, EPR
Characterization	
Experimental Techniques	Flow Chemistry, Organic and Inorganic Materials Synthesis, Colloidal Nanomanufacturing, Microreactor Design and Fabrication, Cyclic Voltammetry, Potentiostatic and Galvanostatic Analyses, Electrodeposition, Electrocatalysis, Electrolysis, Hydrogen Capturing
Programming and Software	Python, MATLAB, COMSOL, ASPEN HYSYS LabVIEW, Origin, SOLIDWORKS, Adobe Illustrator, SIMCA

HONORS & RECOGNITION

Vivian T. Stannett Early Publication Award , Chemical and Biomolecular Engineering Department, North Carolina State University, Raleigh, North Carolina, USA	April 2022
KARAMA's Omid Behbahani Scholarship Award , Tri-State Persian American Association, Cincinnati, Ohio, USA	May 2019
Outstanding Undergraduate Student Award , Awarded merit-based admission to MS. program in Chemical Engineering, Ranked 3rd in the class of 2016, Amirkabir University of Technology, Tehran, Iran	June 2016
Honor Scholar and Double Major Award , Recognized by the office of Brilliant Talents and Olympiads and offered choice of two desired bachelor programs as a distinguished sophomore, Amirkabir University of Technology, Tehran, Iran	January 2014

SELECTED PUBLICATIONS

1. **Batani, F.**; Epps, R. W.; Abdel-latif, K.; Dargis, R.; Han, S.; Volk, A. A.; Ramezani, M.; Cai, T.; Chen, O.; Abolhasani, M., "Ultrafast Cation Doping of Perovskite Quantum Dots in Flow". *Matter* 2021, 4 (7), 2429-2447.
2. Abdel-Latif, K.; **Batani, F.**; Crouse, S.; Abolhasani, M., "Flow Synthesis of Metal Halide Perovskite Quantum Dots: From Rapid Parameter Space Mapping to AI-Guided Modular Manufacturing". *Matter* 2020, 3 (4), 1053-1086.
3. **Batani, F.**; Epps, R. W.; Abdel-latif, K.; Dargis, R.; Bennet, J. A.; Reyes, K. G.; Abolhasani, M., "Autonomous Nanocrystal Doping by Self-Driving Fluidic Micro-Processors". *Advanced Intelligent Systems* 2022, 2200017.

A complete list of 13 publications is available in the following link:

<https://scholar.google.com/citations?user=bHraPToAAAAJ&hl=en>

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Education

- **North Carolina State University, Raleigh, NC (Aug. 2018 – present)**
M.S. Chemical Engineering (Dec. 2020)
Ph.D. candidate Chemical Engineering, Minor in biotechnology, GPA: 3.89/4.00
- **Purdue University, West Lafayette, IN (Aug. 2014 – May 2018)**
B.S. Chemical Engineering, Concentration in Energy and Environment,
Minor in Biochemistry, *Summa Cum Laude*, GPA: 3.89/4.00

Experience

- **Metabolic Engineering of *Caldicellulosiruptor bescii*, Dr. Robert Kelly Lab Hyperthermophile Research Group, NC State University: 2019 – present**
Ph.D. research focused on metabolic engineering of the lignocellulolytic extreme thermophile *C. bescii* to produce desirable volatile products (acetone, ethanol) from plant biomass (such as poplar wood), understanding how *C. bescii* degrades lignocellulose, and identifying desirable characteristics in feedstocks for *C. bescii*.
- **Undergraduate Research, Dr. John Morgan Lab, Purdue: Fall 2016 – Spring 2018**
- **Undergraduate Research, Purdue POWER Lab with Dr. Bryan Boudouris: Fall 2017**
- **Rolls Royce, Materials Technology Center Intern, Indianapolis IN: Summer 2017**
- **Dow AgroSciences, Competitive Intelligence Intern, Indianapolis IN: Summer 2016**
- **Dow AgroSciences, Automation Group Intern, Indianapolis IN: Summer 2015**
- **Rolls Royce, Quality Control Intern, Indianapolis IN: Summer 2014**

Skills

- Anaerobic microbe culture
- Recombinant plasmid construction
- Gibson assembly
- Bacterial genetics (*E. coli*, *Caldicellulosiruptor bescii*)
- Bioreactor operation (2 & 20L scale)
- Protein expression, purification, and characterization
- Tangential flow filtration, cell lysis (chemical, mechanical, enzymatic)
- Epifluorescence microscopy
- DNA & RNA isolation & purification
- Bacterial genome sequencing via Illumina and Oxford-Nanopore
- Transcriptomics - quantitative PCR and RNA sequencing
- Liquid and gas chromatography (HPLC, GC, FPLC)
- Plant biomass processing and composition analysis
- Protein crystallography
- MATLAB, Aspen Plus

Publications

1. **Bing RG, et al. Fermentative conversion of unpretreated plant biomass: A thermophilic threshold for indigenous microbial growth.** (Under review, Sept. 2022).
2. Crosby JR, et al., **Biochemical and Regulatory Analysis of Xylanolytic Regulons in *Caldicellulosiruptor bescii* Reveal Genus-Wide Features of Hemicellulose Utilization.** *Appl Environ Microbiol* (Oct. 2022, In Press)

3. Laemthong T, et al., **Engineering *Caldicellulosiruptor bescii* with Surface Layer Homology Domain-Linked Glycoside Hydrolases Improves Plant Biomass Solubilization.** *Appl Environ Microbiol* (2022).
4. **Bing RG**, Straub CT, et al., **Plant Biomass Fermentation by the Extreme Thermophile *Caldicellulosiruptor bescii* for Co-Production of Green Hydrogen and Acetone: Technoeconomic Analysis.** *Bioresour Technol* (2022).
5. Rodionov DA, et al., **Transcriptional regulation of plant biomass degradation and carbohydrate utilization genes in the extreme thermophile *Caldicellulosiruptor bescii*,** *mSystems* (2021).
6. Zhang K, et al., **Genome-scale metabolic model of *Caldicellulosiruptor bescii* reveals optimal metabolic engineering strategies for bio-based chemical production,** *mSystems* (2021).
7. **Bing RG**, et al., **Thermophilic microbial deconstruction and conversion of natural and transgenic lignocellulose,** *Environ Microbiol Rep* (2021).
8. Straub CT, et al., **Metabolically engineered *Caldicellulosiruptor bescii* as a platform for producing acetone and hydrogen from lignocellulose,** *Biotechnol Bioeng* (2020).
9. Straub CT, et al., **Use of the lignocellulose-degrading bacterium *Caldicellulosiruptor bescii* to assess recalcitrance and conversion of wild-type and transgenic poplar.** *Biotechnol Biofuels* 13, 43 (2020).
10. Lee LL, et al., **The biology and biotechnology of the genus *Caldicellulosiruptor*: recent developments in 'Caldi World'.** *Extremophiles* 24, 1–15 (2020).

Volunteer and Community Service

- Mentor undergraduates in biotechnology research, Spring 2020-present
- Organized and presented biotechnology informational seminar for Grade 9-12 students, Ankeny High School, Iowa, Fall 2019
- Volunteer maintenance of hiking trails, Muir Valley, Kentucky (2014-2019)

Awards

- US NIH Biotechnology Traineeship (T32 GM008776-20, T32 GM133366-01)(2019-2021)
- North Carolina State University Graduate Fellowship (2018-2019)
- Ganiaris Family Chemical Engineering Scholarship, Purdue (2016-2017)

Affiliations

- American Chemical Society: 2014 – present
- American Institute of Chemical Engineers: 2015 – present

References

- Prof. Robert M. Kelly
Department of Chemical and Biomolecular Engineering, NC State University
Email: rmkelly@ncsu.edu, Phone: 919-515-6396
- Prof. Jack P. Wang
Department of Forestry and Environmental Resources, NC State University
Email: jpwang@ncsu.edu, Phone: 919-523-2398
- Additional references available upon request

Andrew S. Clark

3005 Alder Ridge Ln. Raleigh, NC 27603 | asclark@ncsu.edu | 609-947-6513
www.linkedin.com/in/andrew-s-clark

EDUCATION

North Carolina State University **Raleigh, NC**
Ph.D. Candidate in Chemical & Biomolecular Engineering Expected: May 2023
Advised by: Adriana San-Miguel

North Carolina State University **Raleigh, NC**
M.S. in Chemical & Biomolecular Engineering December 2020
GPA: 3.86/4.0; *Summa Cum Laude*

University of Pittsburgh, Swanson School of Engineering **Pittsburgh, PA**
B.S. in Chemical Engineering; Minors Chemistry, Economics December 2017
GPA: 3.88/4.0; *Summa Cum Laude*

WORK EXPERIENCE

San Miguel Lab at NC State **Raleigh, NC**
Graduate Researcher Jan 2019 - Present

- Designed, fabricated, and characterized novel microfluidic devices for high throughput microparticle filtration.
- Identified a robust explanation for microfluidic lobe filtration using ANSYS Fluent simulations.
- Developed an automated image processing algorithm for *C. elegans* neuron degradation quantification in MATLAB.
- Engineered an embedded, microfluidic platform to automatically sort worms based on a computer vision algorithm.
- Spearheaded microfluidic platform development to precisely injure *C. elegans* for neurodegeneration studies.
- Presented experimental results at both in-person and virtual conferences and workshops of >100 people.
- Consulted microfluidic device development for applications including DNA storage and organoid RNA sequencing.
- Collaborated peer-reviewing scientific literature pertaining to microfluidic systems biology topics.

Alcon Laboratories, Inc. **Fort Worth, TX**
Intraocular Lens Research Process Development Intern Summer 2017

- Created new analytical technique to monitor cosmetic defects throughout intraocular lens (IOL) production.
- Assisted with Green Belt Lean Six Sigma project with projected savings over \$100,000.
- Investigated the root cause of significant yield loss occurring in the IOL production process.

Valspar Corporation **Pittsburgh, PA**
Global Technical Center Co-op Engineer Fall 2015

- Organized and revamped a preventative maintenance schedule for Valspar's Global Pilot Plant.
- Streamlined design of experiment and latitude work for new and alternate product introduction.
- Developed of new food-safe polymer product formulations and processes at pilot plant scales.

Valspar Corporation **Garland, TX**
Packaging Co-op Engineer Spring 2015

- Managed and executed project to insert new chilled water lines to solvent reclaim distillation unit.
- Scheduled and completed process safety project work to restore equipment to corporate and OSHA standards.
- Facilitated production of an automated transfer system by designing interlock matrices for Delta-V software.

LEADERSHIP EXPERIENCE

Graduate Research Mentor – San Miguel Lab

Fall 2019 - Present

- Mentored four undergraduate researchers on separate projects involving microfluidics and image processing.
- Designed and led microfabrication and lithography workshops for graduate and undergraduate researchers.
- Supported Future Ingenieros workshops – a program to expose local Latinx high school students (~60) to STEM.

Safety Officer – San Miguel Lab

Summer 2021 - Present

- Designed and developed workflow to accurately track over 100 chemicals used in the laboratory.
- Supervised bi-monthly audits to ensure our lab was OSHA and EHSA compliant.

Teaching Assistant – Chemical & Biomolecular Engineering

Spring 2019 - Spring 2020

- Courses titles: Process Systems Analysis & Control, Design & Analysis of Chemical Reactors, Transport Process II
- Graded weekly homework and exams and led weekly office hours for a three separate classes of over 60-people.
- Facilitated a successful transition to virtual classes and office hours during the COVID-19 pandemic.

Pitt Business Professional Sales Academy

Spring 2017

- 10-week workshop to learn leadership skills in sales – 2nd place finisher in final sales pitch.

AWARDS

- 2021-22 Vivian T. Stannett Graduate Award for Outstanding Early Publication.
- GSA Travel Assistance Award and the College of Engineering Enhancement Fee Award.
- Two-time finalist for Praxair/Lunde Teaching Assistant Award (student-voted exceptional TA award).
- University Graduate Research Fellowship Recipient.

TECHNICAL SKILLS

- **Computer:** AutoCAD, MATLAB, ANSYS Fluent, Python, Microsoft Office, SAS, Inkscape/Adobe Illustrator, SolidWorks, WordPress, Image Processing/Computer Vision, Git, Debugging
- **Lab:** Confocal Fluorescent Microscopy, Microimaging, Microfabrication, Lithography, Microorganism Handling, Microfluidics Device Operation, Embedded Systems

PUBLICATIONS AND PRESENTATIONS

1. **Clark, A.S.**, Kalmanson, Z., Morton, K., Meyer, J. & San-Miguel, A. (2022). An automated, unbiased computer vision platform for dopaminergic degeneration. *In preparation*.
2. **Clark, A.S.**, & San-Miguel, A. (2021). A bioinspired, passive microfluidic lobe filtration system. *Lab on a Chip*, 2021, DOI: 10.1039/D1LC00449B
3. **Clark, A. S.**, Huayta, J., Arulalan, K. S., & San-Miguel, A. (2021). Microfluidic devices for imaging and manipulation of *C. elegans*. *Micro and Nano Systems for Biophysical Studies of Cells and Small Organisms*, 295–321. ISBN: 9780128239902
4. **Clark, A.S.**, & San-Miguel, A. “Passive, microfluidic lobe filtration” MicroTAS 2021, Palm Springs, CA, Oct. 10-14, 2021 (*Poster*)
5. **Clark, A.S.**, & San-Miguel, A. “High-Throughput Microfluidic Microparticle Filtration via Biomimicry of the Manta Ray’s Feeding Mechanism” AIChE Conference 2020. (*Conference talk*)

EDUCATION

University of North Carolina at Chapel Hill
Bachelor of Science in **Polymer Chemistry**, graduated with Honors - May 2018
Aubrey Lee Brooks Merit Scholar & Wood Family Foundation Merit Scholar

North Carolina State University
Master of Science in **Chemical Engineering** – December 2020
Ph.D. in **Chemical Engineering**, expected Ph.D. degree ~ December 2022/January 2023

SKILLS

NMR, GC, DOE, HPLC, GPC/SEC, UV-Vis, Glove Box, DLS, ICP-MS, FIB, SEM, TEM, EDX,
Microfluidics, MS Office, Adobe, Matlab, SolidWorks, LabView.

EXPERIENCE

Department of Chemical Engineering at **NC State University**, Raleigh, NC **August 2018- Present**

Dr. Milad Abolhasani & Dr. Jan Genzer Research Group *Graduate Researcher*

- Conducted research on cross-coupling reactions in continuous flow via network-supported Pd packed bed reactors.
- Synthesized and optimized polymeric networks and gels as supports for catalytically active metals for organic reactions.
- Developed online automated HPLC analysis for sampling of the continuous flow reactions.
- Routinely presented research progress and findings through presentations, posters, and publications.

Becton Dickinson (BD) Technologies, Research Triangle Park, NC **May 2021 – August 2021**
R&D Surgical Product Development *Chemical Engineer-Intern*

- Synthesized and characterized absorbable and degradable polymers and waxes for product development of *in-vivo* surgical products.
- Designed unique *in-vitro* testing methods for the evaluation and screening of samples.

Department of Chemistry at **UNC**, Chapel Hill, NC **December 2016 – May 2018**
Dr. Frank Leibfarth Research Group *Undergraduate Researcher*

- Assisted in graduate research experiments in polymer and organic chemistry.
- Planned and carried out experiments to functionalize commodity polymers post-polymerization.
- Synthesize and test metal-free catalysts in the functionalization of polymers.

Ennis-Flint Research and Development Department **May 2017 – August 2017**
R&D Emulsion Polymerization *Chemist – Internship*

- Conducted independent experiments to reduce coagulum buildup in waterborne latex emulsion polymerizations and improve latex seeds in production for road marking paint and coatings.
- Scaled-up lab reactions to test at the large-scale latex production plant.
- Tested transportation applications, attended business meetings, and engineered new reactions.
- Successfully reduced coagulum buildup in production scale latex reactor by reformulating latex recipe.

- Maintained and updated the student union by painting, plumbing, repairing, building, moving, demolishing, etc.
- Planned building projects and implemented preventative maintenance.

LEADERSHIP

Eagle Scout (2013) – Served as the Senior Patrol Leader of Troop 797 for two years & completed my Eagle Scout Project by leading volunteers, fundraising, budgeting, and project planning.

HOA President (2019-current) – First HOA president for our community of 50 townhouses. Resolve conflicts, plan community engagement events, and create annual budgets.

Lab Safety Officer (2019-current) – Train group members of the Abolhasani lab on general safety and specialized instruments. I oversee safe storage, handling, and organization of toxic, flammable, and corrosive chemicals, and maintaining a safe working environment.

Chemical Engineering Lab TA (2019-current) – Lead and guide the Batch Distillation experiment for undergraduate students to ensure comprehensive understanding of distillation principles.

PUBLICATIONS

Network-Supported, Metal-Mediated Catalysis: progress and perspective

B. A. Davis, J. A. Bennett, K. Efimenko, J. Genzer, and M. Abolhasani, *React. Chem. Eng.*, 2020, **5**, 1892-1902.

Continuous Ligand-Free Suzuki-Miyaura Cross-Coupling Reactions in a Cartridge Flow Reactor Using a Gel-Supported Catalyst

B. A. Davis, J. A. Bennett, M. Ramezani, K. Efimenko, J. Genzer, and M. Abolhasani, *Ind. Eng. Chem. Res.*, 2021, **60**, 9418-9428.

PENDING Poly(β -Cyclodextrin) Network Catalyst for Intensified Hydrogenation in Flow

B. A. Davis, J. A. Bennett, J. Genzer, K. Efimenko, and M. Abolhasani

AICHE Annual Meeting 2021 Oral Presentation: Continuous Ligand-Free Suzuki-Miyaura Cross-Coupling Reactions in a Packed Bed Reactor Using an Easily Synthesized Siloxane Network-Supported Palladium Catalyst

AICHE Annual Meeting 2022 Oral Presentation: Cyclodextrin Network Supported Catalysis in Flow

Summary

Fourth year chemical engineering PhD candidate with a proven ability to adapt to a dynamic, fast-paced environment. My research focuses on the rich and complex fundamental behaviors shown by (i) alternating current (AC) electric field- and (ii) chemical gradient-driven active particles.

Education

North Carolina State University (NCSU), Raleigh, NC Ph.D., Chemical Engineering	Aug 2019 – Present
North Carolina State University (NCSU), Raleigh, NC MS, Chemical Engineering (GPA 3.634)	Aug 2019 – Dec 2021
Worcester Polytechnic Institute (WPI), Worcester, MA BS, Robotics Engineering (GPA 3.6, High Distinction)	Aug 2012 – May 2016

Research Experience

PhD Researcher, NCSU Jan 2019 – Present

Active Particle Propulsion Due to Temporally Asymmetric AC fields

- Investigating electrohydrodynamic effects of temporally nonuniform AC field-driven active particles
- Characterizing and modeling behavior of previously unreported AC field effects
- Introducing additional degrees of freedom for active motion under a single stimulus

Active dispersal of therapeutic agents *via* ultrasimple superdiffusive paste

- Exploring collective behavior of superdiffusive salt paste in chemical gradients
- Assessing spreading and disinfection efficacy on porcine model dermal wounds
- Developing formulation for maximum reach in channels and crevices

Research Experience for Undergraduates, Duke, NCSU, MRSEC May – Aug 2014

Microcube-based Assembly and Actuation of Microbots

- Conducted over 500 hours of research on colloidal assembly designed to produce micro-scale soft robots
- Independently identified successful techniques for transporting microbot with external magnetic field
- Demonstrated novel microbot capture and transport of live yeast cell in test chamber

Presentations and Publications

Coauthor, "AC Electrohydrodynamic Propulsion and Rotation of Active Particles of Engineered Shape and Asymmetry", <i>Curr. Opin. Colloid Interface Sc.</i> 2022.	2022
Poster, "Active Particle Propulsion Due to Temporally Asymmetric AC fields", <i>ELKIN International Symposium on Electrokinetics</i> , Israel	2022
Poster, "New Principles of Active Particle Propulsion Driven by Electrical and Chemical Gradients", <i>Schoenborn Research Symposium</i> , NCSU	2021
Presenter, "Superdiffusive paste from active particles driven by collective phenomena of ionic salt dissolution", <i>ACS Colloid and Surface Science Symposium</i>	2021
Presenter, "Asymmetric AC Field Powered Propulsion of Active Particles", <i>Triangle Soft Matter Workshop</i>	2021
Presenter, "AC Field Powered Propulsion and Light Controlled Steering of Engineered Active Particles", <i>Triangle Soft Matter Workshop</i>	2020
Coauthor, "Sequence-encoded colloidal origami and microbot assemblies from patchy magnetic cubes", <i>Sci. Adv.</i> 2017; 3, e1701108.	2017

Teaching and Leadership Experience

President, Chemical & Biomolecular Engineering Graduate Student Association	Aug 2021 – May 2022
Graduate Recruiting Captain	Jan – April 2022
Faculty Candidate Search Student Committee	Jan– March 2022
Lab Safety Manager, Velev Research Group	Aug 2020 – Present
Graduate Teaching Assistant, Colloid Science and Nanoscale Engineering CHE 596, NCSU	Jan – May 2022
Leadership Development Program Certificate	April 2021
Secretary, Chemical & Biomolecular Engineering Graduate Student Association	Aug 2020 – July 2021
Graduate Teaching Assistant, Undergraduate Thermodynamics CHE 315, NCSU	Aug 2020 – May 2021
Graduate Research Mentor for Undergraduates	Aug 2020 – Present

Work Experience

Embedded Software Specialist, CS Inc, East Hartford, CT Aug 2016 – Jan 2018

- Successfully supported launch of company's first military avionics software verification and validation program
- Encouraged productive relationship with customer through consistent support and punctual delivery of high quality work
- Trained multiple engineers and teams on both commercial and military software verification process and tooling

Skills and Proficiencies

Optical Microscopy, Blender, Solidworks, MATLAB
Highly proficient in thermal evaporation deposition
Kannada, French, German

Xin DONG

NC State | Graduate Research Assistant

📍 2516 Tadley Ct, Raleigh, NC 27603

☎ (440) 541 8225 ✉ xydong@ncsu.edu [in linkedin.com/in/xydong](https://www.linkedin.com/in/xydong)

Optimistic and tenacious fifth year Ph.D. candidate seeking a full-time position relating to machine learning and data analytics. Trained in biomolecular simulations with experience in machine learning, goal-setting, and group collaboration. Excellent communication and technical problem-solving skills.

🎓 EDUCATION

2018-Present	Ph.D. , Chemical Engineering - North Carolina State University, Raleigh, NC
2021	M.S. , Chemical Engineering - North Carolina State University, Raleigh, NC Overall GPA : 3.85/4.00 Expected Graduation : Fall 2023
2018	B.S. , Chemical Engineering - Miami University, Oxford, OH Overall GPA : 3.81/4.00

</> TECHNICAL SKILLS

General	Experienced with high performance computing, Amazon Web Services (AWS), and Linux
Programming & Development	Python (NumPy, Pandas, TensorFlow, Keras, Pytorch), Fortran, MATLAB, SAS Base Programmer Certificate, BASH scripting, git
Simulation & Modeling	Molecular Dynamics, AMBER, VMD
Language	Proficient in Chinese (through ACTFL OPI, Advanced Mid)
Office Tools	LaTeX, Microsoft Office(Word, Excel, PowerPoint)

📁 WORK EXPERIENCE

Aug 2018 Present	Graduate Research Assistant , North Carolina State University, Raleigh, NC PI : Carol K. Hall <ul style="list-style-type: none">> Conducted literature review, developed hypotheses, and designed experiments to generate appropriate datasets to validate hypotheses> Designed and performed atomistic and coarse-grained level simulations of peptides to investigate the mechanism of peptide aggregation and to guide the development of novel biomaterials> Developed new tools in Python and Bash to analyze and visualize large datasets to identify trends in peptide aggregation> Collaborated with multidisciplinary research teams at Georgia Tech and University of Florida to formulate a research plan> Presented simulation results in an accessible manner at meetings, symposiums, and conferences <div style="display: flex; gap: 5px;">Linux AWS HPC Molecular Dynamics AMBER Fortran</div>
Summer 2022	Clinical Pharmacology and Pharmacometrics Intern , Bristol Myers Squibb, Summit, NJ <ul style="list-style-type: none">> Explored and developed multiple machine learning architectures (LSTMs, Transformers, NeuralODEs) for virtual PK/PD (pharmacokinetic/pharmacodynamic) analysis> Determined a best working model to relate dose concentration and virtual patient response> Implemented normalization and standardization preprocessing techniques for models <div style="display: flex; gap: 5px;">Python Tensorflow Keras Pytorch AWS</div>
Summer 2018	Process Engineer Intern , Alsip MiniMill, Alsip, IL <ul style="list-style-type: none">> Performed principal component analysis to determine correlations between process variables (e.g. amount of steam, reel speed, refining power) and paper quality (e.g. basis weight, concora corrugating medium test (CMT))> Determined the effect of alkalinity, temperature, and water hardness of pulp used on stickies (tacky substances found on paper from adhesives and small debris) <div style="display: flex; gap: 5px;">Principal Component Analysis</div>
2015 2018	Undergraduate Research Assistant , Miami University, Oxford, OH PI : Samir Bali Summary : Advanced a method for calculating particle sizes in turbid media

PUBLICATIONS

- > **Dong X**, Liu R, Seroski DT, Hall CK, Hudalla, H, Programming co-assembled peptide nanofiber morphology via sidechain length : Insights from molecular dynamics simulations. *In progress*.
- > Wong K, Robang A, Lint A, Wang Y, **Dong X**, Xiao X, Seroski DT, Liu R, Shao Q, Hudalla G, Hall CK, Paravastu A, Engineering β -sheet peptide coassemblies for biomaterial applications. *Journal of Physical Chemistry Part B*. 2021
- > Seroski DT, **Dong X**, Wong KM, Liu R, Shao Q, Paravastu AK, Hall CK, Hudalla GA. Charge guides pathway selection in β -sheet fibrillizing peptide co-assembly. *Communications Chemistry*. 2020;3(1):1-11. doi:10.1038/s42004-020-00414-w

PRESENTATIONS AND POSTERS

- Nov 2021 Presentation – *Exploring Residue Roles in CATCH Peptide Co-Assembly* presented at the Fall 2021 AIChE Conference
- Nov 2020 Presentation – *Aggregation of Amylin in the Presence of EGCG Using Coarse-Grained Simulations* presented at the Fall 2020 AIChE Conference
- Nov 2020 Poster – *Aggregation of Amylin in the Presence of EGCG Using Coarse-Grained Simulations* presented at the North Carolina State University Biotechnology Training Program Symposium

HONORS AND AWARDS

- 2020-2022 NIH/NCSU Molecular Biotechnology Training Program (MBTP) Fellowship
- 2020 Praxair Exceptional TA award nominee
- 2018 North Carolina State University College of Engineering Graduate Merit Award
- Fall 2017 Benjamin A. Gilman International Scholarship
- 2016 1st place in the AIChE Chemical Engineering for Good Challenge (as a group)

TEACHING ASSISTANT

- > CHE 315 Chemical Process Thermodynamics – Spring 2020, Summer 2020, Fall 2020
- > CHE 311 Transport Processes – Fall 2019
- > CHE 316 Thermodynamics of Chemical and Phase Equilibria – Spring 2019, Spring 2021, Fall 2021

SERVICE ACTIVITIES

- 2020-2021 NC State Chemical Engineering Department, Graduate Recruiting Student Coordinator
- 2019-2020 NC State Chemical Engineering Department Graduate Student Association, Social Chair
- 2015-2017 Miami University AIChE Chapter, Treasurer

MATTHEW A. DORSEY

<https://www.linkedin.com/in/matthewadorsey>

1230 Twin Branches Way, Unit 101
Raleigh, North Carolina 27606

(314) 745 - 3514
madorse2@ncsu.edu

OBJECTIVE

To find a 3-month internship as a Scientific Software Developer or in a field related to Scientific Computing

SUMMARY OF QUALIFICATIONS

- Pursuing a Doctor of Philosophy in Chemical Engineering
- Experience developing custom software to model the behavior of physical systems
- Proficiency working with High Performance Computing clusters via Linux terminal and bash applications
- Strong theoretical background in topics related to physics, chemistry, molecular biology, and mathematics

EDUCATION

Ph.D. in Chemical Engineering

Department of Chemical and Biomolecular Engineering, North Carolina State University

Expected: May 2024

Raleigh, NC

Working Dissertation Title: "Phase Diagrams for Systems of Magnetically-Polarized Square Colloids Under the Influence of Applied-Magnetic and Electric Fields"

M.S. in Chemical Engineering

Department of Chemical and Biomolecular Engineering, North Carolina State University

Dec 2021

Raleigh, NC

Cumulative GPA: 3.56/4.00

B.S. in Chemical Engineering, Minor in Applied Mathematics

College of Computing and Engineering, Missouri University of Science and Technology

Dec 2017

Rolla, MO

Cumulative GPA: 3.68/4.00, *magna cum laude*

RELEVANT PROFESSIONAL EXPERIENCE

[Research Laboratory of Dr. Carol Hall](#) at North Carolina State University

Raleigh, NC

Graduate Research Assistant in Computational Modeling

Since January 2020

- Developed custom molecular simulation software in Fortran 90/95 that uses a Discontinuous Molecular Dynamics (DMD) algorithm to model the physical behavior of atomic and colloidal-scale systems
- Verified custom DMD models by comparing calculated physical parameters (melting point, compressibility factor) to experimental and computational values found in literature
- Established scientific workflow by creating bash scripts to a) submit large numbers of computing jobs with varying initial conditions to High Performance Computing (HPC) clusters and b) collect their results for analysis
- Integrated various numerical and compilation time efficiency techniques which reduced the cumulative computing time of DMD software by approximately 500%, while maintaining its accuracy and performance
- Created java program that converts *.obj* files (generated by CAD software) to *.vtk* legacy format, in order to generate snapshots and movies from molecular simulations with custom objects via OVITO visualization software
- Summarized results of molecular simulations in presentations at research conferences (AIChE) and for publication in research journals

PUBLICATIONS AND PRESENTATIONS

Conference Publications

- **Dorsey, M. A.**, Velev, O. D., Hall, C. K. *Computational Studies on the Structural Properties of Square Colloids with Offset Magnetic Dipoles*. American Institute of Chemical Engineers (AIChE) Conference, Phoenix, AZ, Nov. 2022.
- **Dorsey, M. A.**, Velev, O. D., Hall, C. K. *Simulations of Polarized, Square Microparticles using Discontinuous Molecular Dynamics*. American Institute of Chemical Engineers (AIChE) Conference in Boston, MA, Nov. 2021.

Posters

- “*Computational Studies on the Structural Properties of Square Colloids with Offset Magnetic Dipoles*” at the Schoenborn Research Symposium, North Carolina State University, Raleigh, NC, October 2022.
- “*Computational Studies on the Structural Properties of Square Colloids with Offset Magnetic Dipoles*” at the 10th Annual Triangle Student Research Competition, North Carolina Biotechnology Center, Durham, NC, October 2022.
- “*Optimization of a Novel Biological Method for Synthesizing and Purifying Adipic Acid Using Escherichia coli*” at the Spring SULI Poster Symposium, Berkeley, CA, April 2018.
- “*Determining Differential Curing and Its Effects Within Flexible Cables*” at the Los Alamos National Laboratory Summer Student Symposium in Los Alamos, NM, August 2016.

SKILLS, TECHNIQUES, AND EQUIPMENT

Languages: English (Fluent, Native Speaker), German (Level B1/2, Conversational Fluency and Business Proficiency)

Computer Languages: Fortran 90/95, bash, Java, C/++, MATLAB, Python

Software Programs: OVITO, HTCondor, PyMOL, JMP, Mathematica, SolidWorks, AutoCAD

Molecular Dynamics: Discontinuous Molecular Dynamics (Hard Sphere), Lennard-Jones Fluids (Soft Sphere)

Computing Clusters: Henry2, Open Science Grid (OSG)

TEACHING, LEADERSHIP, AND VOLUNTEER EXPERIENCE

Department of Chemical and Biomolecular Engineering, North Carolina State University Raleigh, NC

Graduate Teaching Assistant Aug 2020 – May 2022

- Assisted Chemical Engineering Department Faculty in facilitating two undergraduate level courses: Transport Phenomena I and Chemical Engineering Process Principles
- Responsible for holding weekly office hours over course material, leading instruction sessions over solving homework problems, writing exam content, and managing Moodle course websites
- Nominated for the Spring 2021, Fall 2021, and Spring 2022 “*Outstanding Teaching Assistant*” award, which is based on student evaluations (six out of ~30 TAs receive this nomination each semester)

Graduate Recruitment Weekend Organizing Committee Spring 2021, Spring 2022

- Worked with a team of 5 - 10 other graduate students to organize a visit weekend for over 30 undergraduate students accepted into the graduate program in Chemical and Biomolecular Engineering at NC State
- Coordinated with faculty, staff, and students to plan events that demonstrate research areas within department and student life, including a graduate student poster session, individual meetings with faculty based on research interests, and social outings with graduate students

Webmaster for 2021 Triangle Soft Matter Workshop May 2021

- Created a virtual poster session environment using Gather.town virtual reality software platform

R. Chris Estridge

(LinkedIn) www.linkedin.com/in/r-chris-estridge

(Address) 278 E Davie St., Raleigh, NC 27601

(Phone) (214)-236-2449, (Email) c_estridge@yahoo.com

TECHNICAL SKILLS

- **Computer Literacy:** Microsoft Office, MATLAB, R, JMP, ImageJ/FIJI, Adobe Illustrator, zUMIs, Seurat, SAMtools, Slingshot
- **Laboratory Techniques/Equipment:** Next Generation Sequencing, Confocal Microscopy, Quantitative Polymerase Chain Reaction, Mammalian Cell Culture, Single-cell RNA-Sequencing, Bioinformatics, Transcriptomics, Quantitative Data Analysis, Gas Chromatography, Mass Spectrometry, Dynamic Mechanical Analysis, Thermal Gravimetric Analysis, Differential Scanning Calorimetry

RESEARCH EXPERIENCE

North Carolina State University, Raleigh, NC, Advised by Dr. Albert Keung (Jan. 2019 – Present)

- Developing techniques for high throughput, high cellular resolution single-cell RNA sequencing while retaining cell spatial information to improve analysis of mammalian tissue samples
- Investigating the role of Matrigel delivery methods and dosage in human cerebral organoid growth and development through immunostaining and single-cell RNA sequencing to improve the cerebral organoid model
- Studying developmental effects of UBE3A absence in human cerebral organoids to gain insight into temporal and cell-type specific outcomes of Angelman syndrome by utilizing bioinformatics tools to analyze Next-Generation Sequencing data

Georgia Institute of Technology, Atlanta, GA, Advised by Dr. Comas Haynes (May – Jul. 2017)

- Designed and performed full-factorial experiment to measure the effects of temperature, media, and anti-agglomerative additives on peracetic acid degradation for ice-slurry chilling in the poultry industry, analyzed data, and discovered no significant peracetic acid degradation under any test condition

The Ohio State University, Columbus, OH, Advised by Dr. Jacques Zakin (Jan. – Dec. 2017)

- Exploited threshold shear stress to enhance heat transfer of a mixed zwitterionic/cationic surfactant solution system in turbulent drag reduction resulting in 80% drag reduction with only 10% heat transfer reduction

INDUSTRIAL EXPERIENCE

Cooper Tire and Rubber Co., Findlay, OH (Aug. 2015 - Dec. 2015, May 2016 - Aug. 2016)

- Performed Dynamic Mechanical Analysis repeatability and reproducibility study using Excel and Minitab
- Identified and reduced major source of variation in new DMA shear specimen preparation method by 50%
- Performed tire chemical reconstruction analysis using thermogravimetric analysis, differential scanning calorimetry, and gas chromatography-mass spectrometry
- Optimized tire cure times resulting in a projected annual savings of \$427,000

CONFERENCE PRESENTATIONS

- **Chris Estridge**, Dilara Sen, Begum Yagci, Jeremy Simon, Albert Keung, *Identifying Cell-Type Composition Differences Between Neurotypical and UBE3A Deletion Human Cerebral Organoids with Single Cell Transcriptomics*, Foundation for Angelman Syndrome Therapeutics Translational Research Symposium, Austin, Texas (December 2-4, 2021)
- **Chris Estridge**, Adam Mischler, Balaji Rao, Albert Keung, *Investigating the Role of Matrigel in Whole Brain Cerebral Organoid Generation*, 4th International Conference on Epigenetics and Bioengineering, Raleigh, North Carolina (October 9-11, 2020)
- **Chris Estridge**, Stephanie Richter, Dan Sabo, Comas Haynes, *Effect of Anti-Agglomerative Agents on the Stability of Peracetic Acid*, SURE Research Symposium, Atlanta, Georgia (July 27, 2017)

TEACHING EXPERIENCE

Department of Chemical and Biomolecular Engineering, North Carolina State University

- Teaching Assistant: Advanced Chemical Engineering Thermodynamics (Aug – Dec 2019)
- Teaching Assistant: Chemical Process Principles (Jan – May 2019)
 - Led recitation section of 50 students to reinforce lecture concepts

Department of Chemical and Biomolecular Engineering, The Ohio State University

- Teaching Assistant: Kinetics (Aug – Dec 2017)

LEADERSHIP AND SERVICE ACTIVITIES

- Undergraduate Student Lab Mentor (January 2021-Present)
 - Manages projects and goals and provides mentorship for four undergraduate students
- Soccer Coach at North Carolina Football Club, Raleigh, NC (Aug. 2021-Present)
 - Coach for U13 Girls team
 - Mentors players, leads training sessions, advises head coach during games
- Chemical Engineering Summer Camp Counselor (June 2021, 2022)
 - Assisted in designing and implementing experiments and facilitated engagement activities to expose high school students to core chemical engineering concepts
- Vice President Internal, Chemical and Biomolecular Engineering Graduate Student Association, North Carolina State University (July 2019-June 2020)
 - Led t-shirt fundraiser and implemented new cost model that resulted in increased profit over previous year to overcome 100% increase in T-shirt cost
- Chemical and Biomolecule Engineering Graduate Recruiting Captain (Jan. 2020-May 2020)
 - Facilitated virtual recruiting of potential 35 CBE students through adopting new digital tools and methods to advertise the CBE program during pandemic
- Student Manager, Oxley's Café, The Ohio State University (Aug. 2014 - Dec. 2017)
 - Supervised and trained 5-7 staff members per shift and trained new hires on equipment and procedures
- Volunteer, Boys & Girls Club of Rockwall County, Rockwall, Texas (Feb. 2012 - Aug. 2016)
 - Supervised, tutored, and mentored 20 1st-8th graders
- Soccer Coach at FC Premier, Dallas, TX (Jun.-Aug. 2014-2016, 2018)
 - Coach for U9-U18 boys teams
 - Led training sessions, advised head coaches during games, and mentored players

AWARDS AND HONORS

North Carolina State University

- Genetics and Genomics Academy (GGA) Summer Mini Grant (Summer 2022)
- NCSU Graduate Student Association (GSA) Conference Travel Award (Spring 2022)
- Genetics and Genomics Academy (GGA) Travel Award (Spring 2022)
- Summer Graduate Merit Award (May 2021)
- First Year Graduate Student Fellowship (Aug. 2018 - May 2019)

Georgia Institute of Technology

- Summer Undergraduate Research in Engineering (SURE) Program (Jun. 2017 - July 2017)

The Ohio State University

- Maximus Scholarship, National Buckeye Scholarship (Aug. 2013 - Dec. 2017)
- Fundamentals of Engineering Honors (FEH) Program (Aug. 2013 - Dec. 2017)
- Second Year Transformational Experience Program (STEP), The Ohio State University (Aug. 2014 - July 2015)

EDUCATION

Aug. 2018 – Present	North Carolina State University, Raleigh, NC (Expected graduation date: December 2023) Ph.D. Department of Chemical and Biomolecular Engineering (G.P.A.: 3.74/4.0)
Aug. 2018 – Nov. 2020	North Carolina State University, Raleigh, NC M.S. Department of Chemical and Biomolecular Engineering (G.P.A.: 3.74/4.0) Thesis: <i>Advancing Tools to Accelerate the Study of Human Neurodevelopment</i>
Aug. 2013 – Dec. 2017	The Ohio State University, Columbus, OH B.S. Department of Chemical and Biomolecular Engineering (G.P.A.: 3.72/4.0) Magna Cum Laude with Honors in Engineering Minor in Business

SOCIETY MEMBERSHIPS

- American Institute of Chemical Engineers (August 2019-Present)
- Society for Biological Engineering (Aug. 2020-Present)
- American Chemical Society (Jan. 2022-Present)

PALLAV K. JANI

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SUMMARY

Collaborative researcher with 4+ years of combined industrial and academic R&D experience in interfacial science, coatings, lubrication, test method development and polymer/metal surface characterization

Experimental & Analytical Skills: Rheological & tribological characterization of gels and coatings; Component interactions in polymeric formulations – isothermal titration calorimetry (ITC), quartz crystal microgravimetry (QCM); Goniometry; Electron microscopy; Confocal laser profilometry; FTIR spectroscopy; UV-vis spectroscopy, Physical vapor deposition of coatings

Computational Skills: MATLAB, Origin, ImageJ, COMSOL, GT-Suite (Friction), MS Office Suite

EDUCATION

North Carolina State University Doctor of Philosophy (Ph.D.), Chemical Engineering GPA – 4.00/4	Raleigh, NC expected December 2023
University of Michigan Master of Science in Engineering (M.S.E), Chemical Engineering GPA 3.69/4	Ann Arbor, MI December 2018
Institute of Chemical Technology Bachelor of Technology (B.Tech.), Oils, Oleochemicals and Surfactants GPA 9.21/10	Mumbai, India May 2017

RESEARCH EXPERIENCE

Graduate Researcher | North Carolina State University, Raleigh, NC September 2019 - present

Advisors: **Saad Khan** and **Lilian Hsiao**

Slip-induced solid lubrication and friction reduction on polymeric substrates

- Demonstrated the adhesion and load-dominant friction dissipation modes of a solid lubricant, erucamide, on different technologically relevant substrates such as PP, LDPE and silicone elastomer
- Correlated the friction reduction benefit of the solid lubricant to the dissipation mode and materials properties of the polymer

Thermodynamic drivers of epoxy-metal oxide adhesion in bisphenol A (BPA)-based epoxy can coating formulations

- Investigated the molecular binding mechanism of epoxy resins with model metal oxides (SnO_2 , Al_2O_3 and Cr_2O_3) using ITC
- Identified the role of surface functional groups on the metal oxide and the polymer backbone in the entropy-driven binding process

Research Assistant | University of Michigan, Ann Arbor, MI October 2017 – April 2019

Advisors: **Johannes Schwank**, **Galen Fisher** and **John Hoard**

Anti-adhesive metal coating to mitigate low temperature (<250°C) turbocharger compressor coking (UM-Ford Alliance Project)

- Developed a sputtered thin transition metal-metal oxide coating to reduce low temperature turbocharger compressor coking by >90%
- Optimized an oil aerosol testing apparatus at Ford R&D to simulate turbocharger deposits and screen metal coatings
- Designed and validated a benchtop apparatus to simulate compressor flow conditions for testing coke adhesion to metal substrates

Student Researcher | University of Michigan, Ann Arbor, MI January – December 2018

Advisors: **Paul Zimmerman** and **Frank Reinhold** (BASF)

Impact of shear on dirt removal in automated washing (Multidisciplinary Design Project with BASF)

- Designed a lab-scale rotating dishwashing setup to quantify dirt removal under shear and implemented a 2^3 factorial DOE testing protocol
- Evaluated the effect of non-ionic surfactant structure on detergency-driven and shear-driven dirt removal regimes

Undergraduate Researcher | Institute of Chemical Technology, Mumbai, India November 2016 – April 2017

Advisor: **Ravindra Kulkarni**

Surfactant assisted co-precipitation protocol to control nanoparticle morphology

- Examined the roles of precursor mixing strategies-dilution and droplet mixing, and surfactant types-cationic and non-ionic, on the morphology of synthesized model BaSO_4 , CaCO_3 and PbCrO_4 nano-precipitates using SEM and XRD analyses

PROFESSIONAL EXPERIENCE

Contact Physics & Tribology Intern | TE Connectivity, Harrisburg, PA June – August 2022

Tribological investigations of surface coatings for stamping tool life improvement and EMI shielding

- Supported ongoing corporate R&D projects to characterize the dry and lubricated friction, wear analyses and identify metal coating failure modes
- Investigated, screened, and developed a rating matrix to down-select promising coatings for product-level testing for two distinct projects in collaboration with multiple business units

Product Development Intern | Ford Motor Company, Dearborn, MI May – July 2019

Friction modeling in diesel engines to predict fuel economy benefits of friction reducing technologies

- Optimized and validated piston-ring friction simulation models in GT-Suite with field trial data (<10% deviation) for 6.7L diesel engines
- Translated friction benefits of ring coatings, low viscosity oils and down-speeding into fuel economy benefits via modified fuel maps

Process Engineering Intern | Adani Wilmar Limited, Mundra, India May – June 2016

- Identified key areas of oil loss by documentation of material flow of palm oil and palm oil-based products
- Proposed optimizations in pressure leaf filtration system to minimize oil loss and increase efficiency of oil refinery

PUBLICATIONS & CONFERENCE PRESENTATIONS

- Adhikari, P.#, **Jani, P.#** et al. “Interfacial contributions in nanodiamond-reinforced polymeric fibers” J. Phys. Chem. B **2021**, 125, 10312-10323 (#co-first authors)
- **Jani, P.** et al. “Frictional shear stress dissipation in slip-induced solid lubricant using tribo-rheometry” The Society of Rheology 93rd Annual Meeting, PF9, **2022**
- **Jani, P.** et al. “Binding interactions at the bisphenol A (BPA) epoxy coating – metal oxide interface: An isothermal titration calorimetry study” American Chemical Society Spring Meeting, 3645016, **2022**
- **Jani, P.;** Farias, B.; Khan, S. A. “Polymer microgels containing nanodiamonds: pH dependent component interactions and rheology” Bulletin of the American Physical Society, 66, **2021**
- Farias, B.; **Jani, P.;** Khan, S. A. “Formation of pickering emulsions using nanodiamonds” Bulletin of the American Physical Society, 66, **2021**
- **Jani, P. K.;** Fisher, G. B.; Uy, D. et al. “Development of a functional coating to mitigate coking in a turbocharger compressor” AIChE Annual Conference, **2019**

AWARDS, LEADERSHIP & ACTIVITIES

Graduate Teaching Assistant | North Carolina State University, Raleigh, NC

- Advanced Process Modeling (Fall 2020), Transport Phenomena (Spring 2021), Polymer Rheology (Spring 2022)
- Finalist for the Linde Teaching Assistant Award for Spring 2021
- Contributed towards drafting a successful research grant proposal on biopolymer surface modification and biodegradability worth \$180K
- Recipient of the Graduate Student Association’s Travel Award to support attendance at the ACS Spring Meeting (2022)
- Recipient of the ‘Division of Soft Matter Meeting Grant’ to support attendance (virtual) at the American Physical Society Meeting (2021)
- Recipient of the ‘Provost’s Doctoral Fellowship’ and ‘Graduate Merit Award’ (2019-2020)

Graduate Student Member

- American Institute of Chemical Engineers (AIChE), American Chemical Society (ACS), American Physical Society (APS), Society of Rheology (SoR)

Event Organizer | Sportsaga, Institute of Chemical Technology, Mumbai, India

- Managed and coordinated a university-level cricket tournament comprising of 16 teams across Mumbai (2014-2016)

Yujin Jang

1910 Entrepreneur Dr. Raleigh, North Carolina 27606, USA
(984) 286-4092 • jangyujin629@gmail.com / yjang4@ncsu.edu • [linkedin.com/in/yujincindy/](https://www.linkedin.com/in/yujincindy/)
NCSU Master of Science in Chemical Engineering, Fulbright 2022-2024

EDUCATION

North Carolina State University – Raleigh, North Carolina Master of Science (MS) in Chemical Engineering	Fall 2022 – Present Fulbright 2022-2024
Austin Language Learning School – Austin, Texas Business English and Intensive English Program	January 2018 – March 2018
University of Central Oklahoma – Edmond, Oklahoma Department of Chemistry, Exchange Student Program	July 2015 – December 2015
University of Hoseo – Asan, South Korea Bachelor of Science Chemical Engineering	March 2013 – February 2017

WORK EXPERIENCE

DuPont (Electronics and Industrial (E&I, Semiconductor Technologies business)) Advanced Cleaning Technology Product Development Engineer	March 2022 – August 2022 Cheonan, South Korea
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- Design, plan, communicate, and participate in a daily test plan for experiments run on the Semi-Works
- Ensure that experimental results are routinely and properly recorded.
- Develop overall product process from laboratory scale to high volume manufacturing scale
- Lead cross-functional teams in problem solving, development of improvement plans and root cause analysis
- Generate technical data according to the requirement

Philip Morris International Lab Analyst	August 2021 – February 2022 Yangsan, South Korea
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- Performed analyses (physical/visual/chemical) on the quality of tobacco, materials, and products
- Calibrated, used, and verified Quality equipment for the accuracy and integrity of the results
- Proposed quality improvement ideas in production and operation
- Investigated critical deviations and proposed quality improvement ideas in production and analyzed the information in projects with influence on product quality

Johnson and Johnson, Consumer Global Technical Operation Engineer	April 2019 – February 2020 Cheongju, South Korea
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- Prepared process validation, verification documentations (OBS/Protocol/Report) for Mixing, Filling, and C&S process
- Performed process verification involving ongoing validation during production of the commercial product
- Monitored and performed testing required for validating equipment, systems, process and utilities
- Outlined and analyzed SOPs related to validation activities
- Measured the pH, viscosity, density of mixing process validation sample

Chemical Engineering Laboratory, University of Florida Research Scientist Internship	May 2018 – December 2018 Gainesville, Florida, United States
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- Improved techniques for measuring concentrations using UV-Vis spectrophotometry and other standard wet lab equipment
- Optimized the design and fabrication of hydrogels loaded with gold nanoparticles
- Hydrogel preparation and characterization, including measuring the thickness and porosity
- Recorded and documented test results using chemistry-specific software programs

Nano-High Polymer Laboratory, Hoseo University**February 2016 – February 2017**

Student Research Scientist

Asan, South Korea

- Gained competence using the micro-pattern imprinting machine, spectrophotometer, electron beam lithography system
- Calculated and set the inputs of speed, load, angle, and depth for the Micro Electro Mechanical System
- Ordered chemicals and prepared reagents for analysis based on laboratory needs

INTERNSHIP**National Institute for International Education (NIIED)****January 2018 – December 2018**

Korea Government Work, English Study, and Travel (WEST) Program

- Korea WEST Program is a joint venture between the United State Department and the South Korean Ministry of Education
- Worked in a professional internship as a research scientist in the Department of Chemical Engineering at University of Florida
- Completed Business English and Intensive English Program at Austin Language Learning School coordinated under the auspices of the United States Department of State's Bureau of Education and Cultural Affairs

RESEARCH EXPERIENCE**Chemical Engineering Laboratory – University of Florida****May 2018 – December 2018*****Design and Fabrication of Hydrogels Loaded with Gold Nanoparticles***

Advisor: Kirk Ziegler, Ph.D., Professor of Chemical Engineering

- Prepared silicone and pHEMA hydrogels through photo-polymerization with different properties and assisted with the synthesis of gold nanoparticles
- Synthesized gold nanoparticles, impregnated them into the hydrogels and measured the responses of the optical spectra to various concentrations of analyte

The designing of Novel Devices for Delivering Ophthalmic drugs

Advisor: Anuj Chauhan Professor, Ph.D., Associate Chair, Chemical Engineering Department

- Prepared contact lenses and nanoparticles to concentrate for controlled release of ophthalmic drugs
- Measured drug uptake and release dynamics as part of the characterization and lens preparation procedure

Nano-High Polymer Laboratory – Hoseo University**August 2016 – November 2016*****Fabrication of Nano-Imprinting Micro-Structure Pattern Using Photo-Curable Polymer***

Advisor: DongCheol, Suh, PhD., Department Chair, Professor of Chemical Engineering

- Gained training in equipment such as UV-Vis spectrophotometer, FT-IR, and micro-pattern imprinting machine
- Consisted of fabrication of micro-structures using a photo-curable polymer

AWARD**Excellent Learnings Award – President of National Institute for International Education****2018**

- Conducted cultural research aimed at improving English proficiency and cultural exchange, which are the core competencies of global talent
- Introduced Korean culture through activities including interviews, discussions, and surveys with people in the United States

Excellent Grader of 'Go Global' International Program Award – Hoseo University**2015**

- Awarded to outstanding students who demonstrate the potential for superior academic performance in an exchange program

Sree Harshita Valli Koduri

Email: harshitakoduri08@gmail.com | <https://www.linkedin.com/in/harshita-koduri-19281720a/> | Phone:(919)6097296

EDUCATION

North Carolina State University, Raleigh, NC Jan 2021 - Present
Master of Science: Chemical and Biomolecular Engineering, GPA- 3.857
Graduate Certificate: Downstream Biomanufacturing

BMS College of Engineering, Bangalore, India Sept 2015 - June 2019
Bachelor of Science: Chemical Engineering, GPA- 3.7

KEY SKILLS

- Centrifugation
- Ultrafiltration/Diafiltration
- Regulatory Affairs
- CRISPR Assay
- ELISA
- Western Blot
- Homogenization
- Protein Purification
- UNICORN
- cGMP
- qPCR
- Soft Lithography
- High Performance Liquid Chromatography(HPLC)
- UV/Vis Spectroscopy
- Quality Auditing, Quality Control
- Gel Electrophoresis
- Cell Culture (CHO cells), Cell Counting
- MATLAB, Microsoft Office

RESEARCH EXPERIENCE & BIOMANUFACTURING EXPERIENCE

Downstream Processing Experience, BTEC, North Carolina State University Jan 2022- Present

- Investigated Chemical, Thermal Stability and Colloidal stability of BSA, GFP and lysozyme at different temperatures.
- Designed a Centrifugation Step for Cell Recovery in the GFP Process based on percent recovery from various flowrates.
- Determined the optimal pressure and number of passes for the homogenization of GFP Cell Paste at manufacturing scale.
- Executed breakthrough runs to determine the dynamic binding capacity of Q Sepharose FF for GFP in clarified Lysate.
- Designed a Chromatography Step for GFP Capture.
- Generated data showing the effect of cross flowrate and transmembrane pressure (TMP) on permeate flux during the ultrafiltration of GFP Q Sepharose FF eluate.

Cell Line Development Research Experience, BTEC, North Carolina State University March 2022- May 2022

- Generated CHO mammalian cell line to produce small antibody fragment (ScFV).
- Screened for best producing clones using limited dilution cloning methods.
- Analyzed protein production using western blot technique.

Research Assistant, North Carolina State University May 2021 – Aug 2022

Liquid Metal-Integrated CRISPR/Cas13 Digital Assay for Ultrasensitive Viral Detection

- Fabricated microfluidic chips of required design using soft lithography.
- Prototyped microfluidic chips using PDMS.
- Injected CRISPR assay through the microfluidic channels and sealed with mineral oil.
- Detected fluorescence signals for the assay in the picomolar range using the 96 well plates and under the microscope in femtomolar range to find the LOD for HIV.

WORK EXPERIENCE

Teaching Assistant, North Carolina State University

Course: Process System Analysis and Control

Jan 2022 – Aug 2022

- Developed test problems and held weekly office hours to aid students with coursework
- Graded exams and homework assignments.

Chemical Engineering Intern, Hetero Drugs Ltd.

July 2018 -Aug 2018

- Designed a process for evaporating solvent during Active Pharmaceutical Ingredient (API) manufacturing.
- Observed various equipment involved in API manufacturing.

ACADEMIC PROJECTS/PAPERS

Synthesis and Characterization of Biodegradable Polymer, Poly (Propylene fumarate), for Biomedical Application

Sept 2018 - May 2019

- Researched the method for synthesis of Polypropylene fumarate (PPF).
- Estimated the cost for laboratory synthesis.
- Formulated the polymer and characterized it using gas chromatography technique.

LEADERSHIP/VOLUNTEER

- Graduate Student Association Social Committee, North Carolina State University
- Volunteered for the NGO-Pasand, Bangalore, India

Yosra Kotb

Raleigh, NC, USA | 919-592-2947 | ymkotb@ncsu.edu | <http://www.linkedin.com/in/yosra-kotb-77301b178>

SUMMARY

Fifth year Chemical Engineering PhD candidate with a meticulous technical aptitude and an innate ability to synthesize, analyze and communicate information. My research interests focus on polymer coatings and adhesives, stratification mechanisms of architectural coatings, and bio-based composites development. Looking for a role where I can transfer my polymer materials knowledge and engineering skills towards my passion for sustainability.

EDUCATION

PhD	Chemical and Biomolecular Engineering North Carolina State University, USA GPA: 4.0	2018-Present
MSc	Chemical Engineering Cairo University, Egypt GPA: 3.9	2014-2017
BSc	Petrochemicals and Petroleum Engineering. Major: Petrochemicals Engineering Cairo University, Egypt GPA: 3.85- First class distinction with Honors	2009-2014

RESEARCH EXPERIENCE

PhD researcher , North Carolina State University	<ul style="list-style-type: none">Investigating the structure-property relationships pertaining to the corrosion protection of organic coatings on metalsExploring the adhesion origins of multiple organic coating resins on metallic substratesAnalyzing the self-stratification performance of binary latex blends in waterborne architectural coatingsBuilding an electrochemical and optical characterization toolbox for the detection of filiform corrosion on powder coated aluminum alloysPatented a new class of sustainable biopolymers-based composites reinforced with dendritic colloidal particlesDeveloped and tested superhydrophobic and icephobic coatings made from nanofibrillated polymer colloidal particlesLed the conception and preparation of 3 accepted/funded research proposalsAchieved excellent collaborations with multiple industrial partners (BASF, Behr & Eastman) leading to projects funding/extension	2018-present
Graduate Research Intern , Metal Packaging Coatings, Eastman Chemical Company	<ul style="list-style-type: none">Developed a new accelerated test protocol for high flexibility polyester can coatings to match the real-time pack test resultsWorked on electrochemical characterization of can coatings degradation using electrochemical impedance spectroscopy as well as modeling equivalent electric circuit models to interpret the results	October 2021- January 2022
Research & Development Intern , Performance Coatings Group, The Sherwin Williams Company	<ul style="list-style-type: none">Assisted in the development of a clear matte UV-cured top coating for hardwood flooringTested and optimized several pigments and additives to achieve required viscosity, gloss, and scratch resistance	May- July 2021
Graduate Research Assistant , Cairo University	<ul style="list-style-type: none">Developed a COMSOL mathematical model describing the electrochemical conversion of CO₂ into CH₃OH	2014-2017

TEACHING & LEADERSHIP EXPERIENCE

Teaching Assistant , North Carolina State University	<ul style="list-style-type: none">Assisted in teaching undergraduate and graduate level Thermodynamics courses in chemical engineeringAdvised and trained 4 M.Sc. and 1 undergraduate lab research students	2018- Present
Assistant Lecturer , Cairo University	<ul style="list-style-type: none">Taught and assisted in teaching 4 undergraduate chemical engineering courses: Applied electrochemistry and corrosion, Heat transfer, Organic chemistry, and Freshman chemistryPrepared course material including lectures, exams, assignments, and practice problemsLed weekly laboratory and/or tutorial sessions for groups of 40-60 students	2017-2018
Teaching Assistant , Zewail City of Science and Technology	<ul style="list-style-type: none">Taught and assisted in teaching 4 undergraduate environmental engineering courses: Phase equilibria, Mass and energy balances, Heat transfer, and Renewable energy systemsLed weekly tutorial sessions for groups of 30-40 students	2015-2017

PUBLICATIONS & SELECTED CONFERENCE PROCEEDINGS

- Kotb, Y.**, Serfass, C.M., Cagnard, A., Houston, K.R., Khan, S.A, Hsiao, L.C., Velev, O.D. (2022) Molecular structure effects on the mechanisms of corrosion protection of model epoxy coatings on metals. *Submitted*
- Williams, A.H., Roh, S., **Kotb, Y.**, Velev, O.D. (2022) Superhydrophobic and Anti-Icing Coatings Made of Hierarchically Nanofibrillated Polymer Colloids. *Macromolecular Rapid Communications*
- Kotb, Y.**, Velev, O.D. (2022). Novel Principles of Fabricating High-performance Sustainable Biopolymer Films Hierarchically Reinforced with Dendricolloids. *96th ACS Colloid and Surface Science Symposium, CO, USA*
- Kotb, Y.**, Khan, S.A., Hsiao, L.C., Velev, O.D. (2022). Correlating the Surface Energetics, Molecular Adhesion Characteristics, and Stability of Epoxy-Phenolic Coatings on Metals. *96th ACS Colloid and Surface Science Symposium, CO, USA*
- Serfass, C.M., **Kotb, Y.**, Smith, K.M., Houston, K. R., Khan, S. A., Velev, O. D., Hsiao, L. C. (2022). Microstructural Defects of Epoxy-Phenolic Polymers on Metal Substrates during Acidic Corrosion. *ACS Applied Polymer Materials*, 4(5), 3196-3204
- Kotb, Y.**, Cagnard, A., Houston, K.R., Khan, S.A., Hsiao, L.C., Velev, O.D. (2022). What makes epoxy-phenolic coatings on metals ubiquitous: Surface energetics and molecular adhesion characteristics. *Journal of Colloid and Interface Science*, 608(1), 634-643
- Kotb, Y.**, Velev, O.D (2021). A New Class of Biodegradable, Tough, and Clear Polysaccharide Films Reinforced with Nanofibrillated Chitosan. *ACS Spring*, virtual
- Kotb, Y.**, Fateen, S. E. K., Albo, J., & Ismail, I. (2017). Modeling of a Microfluidic Electrochemical Cell for the Electro-Reduction of CO₂ to CH₃OH. *Journal of The Electrochemical Society*, 164(13), E391-E400
- Kotb, Y.**, Fateen, S.K., Albo, J., Ismail, I. (2016). Modeling of the Electrochemical Reduction of CO₂ to Methanol in a Micro Flow Cell. *COMSOL conference, Munich, Germany*

PATENTS

Velev, O.D., **Kotb, Y.** (2022). Biodegradable biopolymer films. US patent pending No. 17/548,569

TECHNICAL SKILLS

- SEM| EDX| AFM| Confocal and optical microscopy| Mechanical testing| EIS| TGA| DSC| DMA| FT-IR| Rheometry| Goniometry| Tensiometry| DLS, ELS| UV-Vis spectroscopy| Oxygen and water vapor permeability characterization
- MATLAB| COMSOL Multiphysics| Minitab| JMP

AWARDS & PROFESSIONAL DEVELOPMENT

- Honorable mention in Graduate student/Postdoc Microscopy, Envisioning Research Contest, 2022, NC State University
- Recipient of the Graduate Student Association Travel Assistance Award, Spring 2022, NC State University
- Recipient of the College of Engineering Travel Award, Summer 2022, NC State University
- Finalist in Praxair Exceptional Teaching Assistant award, Spring 2019, NC State University
- Course in "Corrosion: Fundamentals and Experimental Methods", Fall 2021, Ohio State University

Junchen Liu

Telephone: (765)-838-9538; e-mail: jliu59@ncsu.edu;

Education

Ph. D. in Chemical Engineering expected Aug 2023
North Carolina State University, Raleigh, NC
Thesis: "CO₂ capture, utilization and mitigation via ethane and alkylbenzene oxidative dehydrogenation"

B. S. in Chemical Engineering May 2018
B. S. in Chemistry May 2018
Purdue University, West Lafayette, IN

Research Experience

Redox ODH of alkylbenzene – Eastman Funded Project 2020-2023

- Designed and improved the lab-scale multiphase reactor for alkylbenzene dehydrogenation setup
- Increased the single pass yield of alkenylbenzene by >40%
- Estimated a process energy requirement reduction by >50% via Aspen Plus Modeling
- Utilized factorial design to optimize catalyst composition to enhance CO₂ resistance of the catalysts
- Compiled data and formally presented data with Eastman Chemical Co. monthly
- Completed preliminary process design and equipment procurement for establishing a scale-up unit for proof-of-concept process demonstration

Super-equilibrium methane steam reforming pilot plant 2022

- Built a scale-up 1,000 SCF/day pilot plant for methane reforming with teams
- Assessed the pressure swing the temperature swing capability of the reactor systems
- Assisted in procurement of the setup equipment

CO₂ Capture and Utilization with Ethane Cracking via Molten Carbonates 2019-2020

- Developed molten-salt based process that achieved 90% CO yield from CO₂ utilization
- Determined 44.6% energy compared to conventional CO₂ capture-and-utilization approach via Aspen Plus Modeling
- Constructed an corrosion resistant molten salt reactor and tested over 100 hours

Direct Arylation Polymerizations 2016-2017

- Developed a thieno-benzo-isindigo based polymer synthesis route via Direct Arylations
- Achieved up to 121.6 kDa high molecular weight polymers with low PDI (6.5)

Optimization of O₂ plasma-assisted oxidation of Fe₂O₃ thin film 2016-2017

- Developed a synthesis route by using O₂ plasma instead of O₃ for Fe₂O₃ thin film growth
- Optimized O₂ purging rate for enhance uniformity of the thin film surface

Work Experience

Process Engineering Intern, packaging 2018
Western Digital

- Explore the use of dual laser setup for wafer cutting to replace the conventional blade cutting method
- Use Design of Experiment with JMP to optimize the dual laser wafer cutting passing rate
- Analyzed and identified the cause of defects on the silicon wafer with microscope
- Developed a software for invoice processing with Python to improve invoice process rate

Quality Control Intern, 2015
W. L. Gore & Associates

- Performed FT-IR on 200+ polymer samples to improve product final pass yield
- Performed aging test to predict the materials' life expectancy

Leadership Experience

Laboratory Safety Officer

2020-2022

- Oversaw operations for Dr. Fanxing Li's group at North Carolina State University
- Led safety trainings and organize safety notice to educate more than 10 personnel (undergraduates/graduates)
- Established framework for monthly cleanliness point person to ensure lab cleanliness
- Developed single-point-of-contact framework for characterization techniques to improve group's efficiency and knowledge retention

Undergraduate Mentor (2 mentored, 1 in progress)

2019-2022

- Trained undergraduates for dehydrogenation experiment operations and statistical data analysis

Entrepreneurial Experience

Venture Opportunity Analyst, MBA 572

2022

- Collaborated with a start-up company to assess risk for current business proposals on participation in carbon inssetting market
- Conducted 15+ interviews with CPG companies stakeholders to estimate the value-adds of the carbon neutral labeling
- Perform cost and benefit analyses via statistical analyses on continuous and categorical data to minimize risk
- Devised recommendations and solutions for current proposals

Patents

1. Filed Provisional. "Redox Catalysts and Processes For Efficient Oxidative Dehydrogenation Of Alkylaromatics" Liu, J; Li, Fanxing, Filed: June 3rd, 2022, Under Review with Application Number: 63/348,550

Manuscripts and Publications

1. **Liu, J.** & Li, F. Mixed Oxides as Multi-Functional Reaction Media for Chemical Looping Beyond Combustion *ChemComm, in draft*
2. **Liu, J.**, Yusuf, S., Jackson, D, Martin, W., Chacko, D., Vogt-Lowell, K., Neal, L., & Li, F. Redox Oxide@Molten Salt as a generalized catalyst design strategy for oxidative dehydrogenation of ethane via selective hydrogen combustion Ru-promoted perovskites as effective redox catalysts for CO₂ splitting and methane partial oxidation in a cyclic redox scheme. *Applied Catalysis A: General, in press*
3. **Liu, J.**, Gao, Y., Wang, X., & Li, F. (2021). Molten-salt-mediated carbon dioxide capture and superequilibrium utilization with ethane oxidative dehydrogenation. *Cell Reports Physical Science, 2(7)*.

Coauthored articles for contribution on X-ray photoelectron spectroscopy available upon request

Selected Honors and Awards

- North American Catalysis Society Richard J. Kokes Travel Award 2022
- Southeast catalysis society SE Catalysis Poster Award 2019
- North Carolina State University Graduate Merit Award 2018
- Purdue University Summer Undergraduate Research Fellowship Recipient 2017
- Purdue University Discovery Park Undergraduate Research Internship Recipient 2016

Professional Services and Associations

- American Institute of Chemical Engineers (AIChE), the American Chemical Society (ACS)
- Treasurer, Tau Beta Pi Engineering Honor Society, Research Triangle Park
- Guest Editor, "Advanced Catalyst Synthesis and Characterization" Special Issue of the *Recent Progress in Materials*

Skills and Interest

- Catalyst Design
- XPS
- XRF
- TGA-DSC
- *In-situ* FTIR
- Raman Spectroscopy
- *In-situ* XRD
- Python
- Design of Experiment
- Venture Analysis

Zvikomborero Machikiti

Raleigh, NC | zmachik@ncsu.edu | +1-484-541-9788 | <https://www.linkedin.com/in/zviko-mac-2aa35ba4/>

OBJECTIVE

Exceptionally focused, motivated, innovative, and detail-oriented PhD student seeking a summer internship in R&D. Wide breadth of knowledge in industrial chemical processes with emphasis on polymer synthesis and characterization, and excellent research and data analysis skills. Able to multitask effectively, and brilliant in handling high-pressure and fast-paced environments.

EDUCATION

North Carolina State University – Raleigh, North Carolina, USA

- Doctor of Philosophy in Chemical and Biomolecular Engineering May 2024
- Master of Science in Chemical Engineering December 2021

Lafayette College – Easton, Pennsylvania, USA May 2019

- Bachelor of Science in Chemical Engineering
- Minor in Economics with a Concentration in Finance

RESEARCH EXPERIENCE

Graduate Research Assistant - North Carolina State University August 2019 - Current

- Establishing simple, robust methods to tailor adhesion at the polyester/polyamide interface by adding organic species with the goal of reducing energy requirements in splitting bonded polymers in collaboration with Nonwovens Institute
- Extruding various bicomponent fibers and determining the degree of splittability of bicomponent fibers used for manufacturing end products such as carpets, blankets, and towels
- Designing a polymer synthesis experimental procedure to produce a poly(R-alt-maleic anhydride) with a yield greater than 95% in less than five hours. The polymer is valuable in tailoring adhesion between polyester/polyamide

EXCEL Research Scholar - Lafayette College December 2017 - August 2018

- Optimized the co-solvent conditions for the supercritical fluid extraction of betulin from birch bark with a yield of 90%
- Developed the method for identification of betulin on the Supercritical Fluid Chromatogram
- Performed polymerization synthesis in the presence of a greener and cleaner solvent, supercritical carbon dioxide. Research project resulted in biopolymers with applications such as producing utensils, and storage bags

TEACHING EXPERIENCE

Chemical Engineering Lab I Teacher Assistant - North Carolina State University August 2020 - May 2022

- Conducted training in using lab equipment, and lab safety resulting in zero safety emergencies and accidents
- Implemented design of experimental apparatuses and managed lab equipment leading to no malfunctioning of equipment

Global Energy Challenge Laboratory Assistant - Lafayette College August 2017 – May 2019

- Organized laboratory equipment for biodiesel generation experiments for the class resulting in 100% success rate in experiments execution
- Monitored and assisted students in carrying out experiments, and created the grading rubric of 50 exams

PUBLICATIONS AND CONFERENCE PRESENTATIONS

- Machikiti, Z., et al. (2022). *Controlling PA6/PET adhesion to facilitate interfacial fracture*. European Polymer Journal, 171, 111196.
- Machikiti, Z., et. al. *Controlling PA6/PET adhesion to facilitate interfacial fracture*. IDEA22, Miami Beach, FL, 2022.
- Machikiti, Z., et. al. *Controlling PA6/PET adhesion to facilitate interfacial fracture*. RISE, Raleigh, NC, 2022.
- Machikiti, Z., et. al. *Development of Green Production of Biopolymers*. AIChE Annual Meeting. Pittsburg, PA, 2018.

SKILLS

Experimental/Chemical techniques

- Experiment design
- Expert in polymer synthesis
- Extrusion process
- Material characterization

Software skills

- Microsoft office
- MATLAB
- Aspen
- TRIOS
- Minitab
- AutoCAD
- Origin
- Polymath

Soft skills

- Excellent communication ability
- Excellent interpersonal skills
- Competent organizational skills
- Team player
- Strong verbal and presentation skills
- Creative
- Proactive
- Flexible

ACTIVITIES/ CLUBS

- Acapella, Choir, Investment Club, Peer Advisor, Librarian, Chess, Intramural Volleyball, Intramural Soccer, Frisbee

William E. Martin
wemartin@ncsu.edu – (252) 481-1199

Permanent Address
824 Lexington Dr.
Greenville, NC, 27834

Local Address
1004 Chapanoke Rd.
Raleigh, NC, 27603

Education

- MS Thesis in Chemical Engineering** May 2023
Thesis: “CO₂ capture and utilization via chemical looping”
North Carolina State University
- B.S. Chemical Engineering** May 2021
Concentration in Sustainable Engineering, Energy and The Environment
Minors - Business Entrepreneurship and Environmental Sciences
North Carolina State University
- Study Abroad** Dec 2018
Introduction to Sustainable Engineering
Reykjavik University

Work Experience

- R&D Lab Technician Intern, Domtar Personal Care** Fall 2018
- Completed various daily research and quality tests on Domtar current and future products
 - Was able to test a variety of different theories after working closely with some of the lead research scientists and offer input to help further research

Research Experience

- Thermophotocatalysis Dry Reformation of Methane** 2019-2020
Undergraduate Research Assistant – Li Research Lab
- Learned the basics of working within a university lab
 - Dealt with chemical inventory and safe storage of chemicals
 - Synthesized and tested required mixed-metal oxides
 - Assisted and operated in the design of a thermo-photo reactor
- DFT Predicted Perovskites for Syngas Production via Chemical Looping** 2020-2021
Undergraduate Research Assistant
- Synthesized, characterized, and tested a variety of perovskites and reported data to DFT collaborators to fine tune DFT calculations
 - Collaborated in the designing of perovskites to achieve >90% both CH₄ and CO₂ conversions at low temperatures
- CO₂ Utilization and Conversion Through Dry Reformation of Methane via Ruddlesden-Popper and Perovskite Phase-Based Materials in a Chemical Looping Scheme for Syngas Production** 2021-Present

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Raleigh, NC, 27603

- Differentiating between the two types of catalysts and their catalytic functions through redox testing and different characteristic techniques
- Able to have a flexible Oxygen Carrier and CO₂ carrier, allowing the tuning of H₂:CO ratio for downstream industrial needs
- Achieved >85% CO₂ capture and CH₄ conversion within the first 20 cycles

Super-Equilibrium Methane Steam Reforming Pilot Plant

2022-Present

- Assisted in the assembling of the reactor as well as procurement of materials needed
- Process engineer role and data analysis/reporting
- Solo operation of the plant

Skills

- Proficient in Microsoft Excel
- Able to operate and maintenance gas chromatography, mass spectrometer, and BET instruments
- Design gas line configurations for specific experimental needs
- Trained for X-ray Diffraction Analysis, both ex-situ and in-situ
- Versed in ASPEN computing
- Work well with other group members
- Able to meet deadlines efficiently and on time

Academic Services

CHE 450 Grader

2022

- Worked with the professor and other TA/graders for grading of tests/homework
- Assisted students through questions regarding the class in general and content

Affiliated Publications

1. Liu, J., Yusuf, S., Jackson, D., **Martin, W.**, Chacko, D., Vogt-Lowell, K., Neal, L., & Li, F. Redox Oxide@Molten Salt as a generalized catalyst design strategy for oxidative dehydrogenation of ethane via selective hydrogen combustion Ru-promoted perovskites as effective redox catalysts for CO₂ splitting and methane partial oxidation in a cyclic redox scheme. *Applied Catalysis A: General*
2. Iftikhar, S., **Martin, W.**, Gao, Y., Yu, X., Wang, I., Wu, Z., Li, F. LaNi_xFe_{1-x}O₃ as flexible oxygen or carbon carriers for tunable syngas production and CO₂ utilization. *Catalysis Today*
3. Iftikhar, S., **Martin, W.**, Wang, X., Gao, Y., Liu, J., Li, F. Perovskite nanocomposites as effective oxygen carriers for CH₄ partial oxidation and CO₂ splitting in a cyclic redox scheme. *Nanoscale*
4. **Martin, W.**, Iftikhar, S., Brody, L., Li, F. Tunable syngas production and CO₂ utilization via ruddlesden-popper and perovskite phase-based catalysts. *In Draft*

Sarah E. Morgan

NDSEG Fellow - Department of Chemical & Biomolecular Engineering - North Carolina State University - Raleigh, NC
(618)402-3005, sesmit28@ncsu.edu

HIGHLIGHTS

- Integration of metal-organic framework (MOF) catalysts onto fabrics for personal protection against toxic chemicals
- Introducing vapor-based, industrially relevant roll-to-roll methods for synthesizing MOF coated textiles
- Product management, procuring funds, market research, and VOC development for textiles developed in lab
- Three years of undergraduate student management: 5 total students, 3 in parallel
- Project lead for Defense Threat Reduction Agency research: monthly meetings, reports, research presentations

EDUCATION

- 2018 – Present** **North Carolina State University, Raleigh, NC,**
Ph.D. Chemical Engineering, GPA 3.8/4.0, (anticipated Spring 2023)
- 2013 – 2018** **University of Kentucky, Lexington, KY**
B.S. Chemical Engineering + B.S. Materials Engineering, GPA: 3.9/4.0

EXPERIENCES

- 2018 – Present** *Research assistant* (Parsons' lab), North Carolina State University, Raleigh, NC
- Developing benign methods for MOF growth on polymer fibers and films for toxic chemical adsorption and degradation
 - Thin film MOF formation on polymer fibers and planar substrates
 - Safety officer 2019-2021
- 2022 Fall** *I-Corps entrepreneurial lead*, North Carolina State University, Raleigh, NC
- Developing VOC data via customer interviews
 - Presenting product pitches to potential stakeholders
- 2017 Summer** *R&D intern*, Nestlé Purina, St. Louis, MO
- Assisted pilot plant trials on extruder, dryer, and batch operations
 - Mathematical modeling, innovation, and capital investment projects
- 2017 – 2018** *Research assistant*, Hummingbird Nano SBIR, Lexington, KY
- Prepared metal oxide nanoparticle doped polymers to enhance optical properties
- 2016 Summer** *Summer undergraduate research fellowship (SURF)*, National Institute of Standards and Technology (Dr. Shin Muramoto), Gaithersburg, MD
- Supported development of a fingerprint dating methods using ToF-SIMS
- 2015 Summer** *Chemical engineering intern*, FP International, Hopkinsville, KY
- 6 R&D projects improving safety, increasing productivity, and developing new products
- 2014 - 2015** Undergraduate researcher (Agouridis' lab), University of Kentucky, Lexington KY
- 2014 - 2017** Undergraduate TA for General Chemistry 2, Lexington, KY

HIGHLIGHTED SKILLS

Analytical characterization and other: Scanning electron microscopy, X-ray diffraction, Brunauer-Emmett-Teller, Fourier transform infrared spectroscopy, Ultraviolet-visible spectroscopy, X-ray photoelectron spectroscopy, mechanical characterization, atomic layer deposition

Software: Origin, Adobe Illustrator, Image J, Microsoft suite

INTELLECTUAL PROPERTY

1. "MOF-FABRIC COMPOSITES AND METHODS OF MOF-FABRIC COMPOSITE SYNTHESIS," U.S. Provisional Patent No. 63/279,923 Filed on November 16, 2021.

Sarah E. Morgan

PUBLICATIONS

1. **Sarah E. Morgan**, Morgan L. Willis, Gregory W. Peterson, John J. Mahle, Gregory N. Parsons “Green MOF-fabrics: Benign, scalable sorption-vapor synthesis of catalytic composites to protect against phosphorus-based toxins.” (ACS Sustain. Chem. & Eng., **2022**, 10.8, 2699-2707) DOI: 10.1021/acssuschemeng.1c07512
2. **Sarah E. Morgan**, Andie M. O’Connell, Anton Jansson, Gregory W. Peterson, John J. Mahle, Tim B. Eldred, Wenpei Gao, Gregory N. Parsons, “Stretchable and Multi-Metal–Organic Framework Fabrics Via High-Yield Rapid Sorption-Vapor Synthesis and Their Application in Chemical Warfare Agent Hydrolysis” (ACS Appl. Mater. Interfaces, **2021**, 13.26, 31279-31284) DOI: 10.1021/acsami.1c07366
3. **Sarah E. Morgan**, Morgan L. Willis, Golnaz Dianat, Gregory W. Peterson, John J. Mahle, Gregory N. Parsons, “Toxin-Blocking Textiles: Rapid, benign, roll-to-roll production of robust MOF-Fabric composites for organophosphate separation and hydrolysis” *Submitted*

HONORS AND AWARDS

2022 Chancellor’s Innovation Fund. \$50k awarded to pursue commercialization of IP. Prepared white paper, full proposal, and presented product pitch to local investors.

2022 Exemplary Impact and Relevance to DoD Research Objectives. 2022 DoD National NDSEG Fellows Conference

2021 Materials Advances Best Poster Award. EuroMOF 2021

2020 DoD National Defense Science and Engineering Graduate (NDSEG) Fellow. Three-year, full support of PhD research including stipend (\$38K/yr), travel (\$5K), and DoD mentor

2018 Various Awards. NCSU University Graduate Fellow (\$4K), NCUS Graduate Merit Award (\$2K)

2015 2nd Place Oral Presentation. American Society of Mining and Reclamation National Conference

2013-2017 Various Awards. Scholarships (~\$4K/semester) from the University of Kentucky for undergraduate studies

SELECTED TECHNICAL PRESENTATIONS

1. **Sarah E. Morgan**, Morgan L. Willis, Golnaz Dianat, Gregory W. Peterson, John J. Mahle, Gregory N. Parsons “Organophosphate chemical warfare agent degradation and filtration using metal-organic framework fabrics synthesized by a rapid, benign, scalable process” Oral, Chemical and Biological Defense Science & Technology (CBD S&T) Conference, San Francisco, CA, December **2022**, planned
2. **Sarah E. Morgan**, Andie M. O’Connell, Morgan L. Willis, Carwynn D. Rivera, John J. Mahle, Gregory W. Peterson, Gregory N. Parsons “MOF-fabric for chemical warfare agent protection: journey from toxic, slow, batch synthesis to benign, rapid, continuous production” Oral, Schoenborn Research Symposium, Raleigh, NC, October **2022**, planned
3. **Sarah E. Morgan**, “Metal-organic framework fabric composites for degradation of chemical warfare agents” Oral/poster, 2022 DoD National NDSEG Fellows Conference, Boston, MA, July **2022**.
4. **Sarah E. Morgan**, Andie M. O’Connell, Anton Jansson, Gregory W. Peterson, John J. Mahle, Wenpei Gao, Tim B. Elrod, Gregory N. Parsons “Rapid vapor crystallization of stretchable MOF-fiber composites for chemical warfare agent hydrolysis” Oral/poster, EuroMOF 2021, virtual, September **2021**.
5. **Sarah E. Morgan**, Heather F. Barton, Gregory W. Peterson, Natalie L. Pomerantz, Gregory N. Parsons “Multiple methods for nucleation and growth of MOFs on polymer surfaces and fiber mats”, Poster, 2019 DTRA Science Review for Surface Science and Multifunctional Materials, Aberdeen Proving Ground, MD, September **2019**

CURRENT RESEARCH

1. **Sarah E. Morgan**, Rachel S. Bang, Morgan L. Willis, Gregory N. Parsons, “MOF-paper nonwoven composites for absorption of oil, microplastics, and other contaminants from water”
2. Rachel A. Nye, Nicholas M. Carroll, **Sarah E. Morgan**, Gregory N. Parsons, “Vapor-Phase ZIF-8 Growth on Fibrous Polymer Substrates and Quantitative Analysis of Metal Oxide-to-MOF Conversion Reactions”

SNEHA MUKHERJEE

512 Tartan circle, Apt 21, Raleigh, NC, US | +1-984-255-3376 | smukhe22@ncsu.edu

OBJECTIVE AND AREAS OF INTEREST

PhD student with research experience in wearable sweat sensors, paper microfluidics based sensors, lateral flow assays, biological assays for health monitoring. Also worked on advanced 2-D materials, nanomaterials/nanofibers for supercapacitors, air filters and biomedical applications, leaching and CO₂ sequestration.

EDUCATION

North Carolina State University, Raleigh, US	Aug'19 - Present
PhD – Chemical and Biomolecular Engineering	GPA:3.92/4
MS- Chemical and Biomolecular Engineering (on the way to PhD)	Dec'21
Indian Institute of Technology, Kharagpur, India	May'18
Master of Technology -Chemical Engineering	GPA: 9.1/10
BMS College of Engineering (BMSCE), Bangalore, India	May'16
Bachelor of Engineering -Chemical Engineering	GPA: 9.54/10

RELEVANT RESEARCH EXPERIENCE

‘Sequential Layering of DNA on Microfluidic Paper Device’ – funded by NSF

Advisors: Dr. Orlin D. Velev, NCSU

PhD Candidate Aug'21- Present

- Explore the use of paper microfluidic manipulation to spatially pattern or partition different fractions of a DNA at discrete, specific spatial locations.
- Exploring the colloidal properties of DNA and DNA bound on nanoparticles through dynamic light scattering.

‘Wearable sensors for health monitoring from sweat’ – funded by AFRL

Advisors: Dr. O. D. Velev and Dr. M. D. Dickey, NCSU

PhD Student Jan'20- July'21

- Developing a lateral flow immunoassay platform for analyte (cortisol, potassium ions) detection in sweat, that functions under the novel, non-invasive simultaneous action of osmosis (for sweat sampling from skin) and evaporation (for sustaining continuous flow).
- Testing the patches on human subjects on rest and undergoing exercise to quantify analyte levels in their body.

OTHER PROJECTS & INTERNSHIPS

- ‘2D materials beyond graphene’ - Advanced Functional Materials, Council for Scientific & Industrial Research- National Metallurgical Laboratory. Oct'18-Jul'19
- ‘Biomimetic Synthesis and Characterization of Nanocomposites/Nanofibers for medicinal or energy applications’- Advanced Functional Materials, Council for Scientific & Industrial Research- National Metallurgical Laboratory. Jun'18-Jul'19
- ‘Demineralisation of High Ash Coal’ -Tata Steel R&D Centre & IIT Kharagpur Jun'17- Apr'18
- ‘Design and fabrication of a reactor for mineral waste carbon sequestration’- BMSCE, Bangalore Sept'15-May'16
- Intern, Indian Oil Corporation Limited, Haldia Refinery, India Jun-Jul'15
- Graduate Research Intern, R&D, Tata Steel Limited, India Jun'17-Apr'18

PUBLICATIONS

- S.Mukherjee, S.P. Salazar, T.Saha, M.D.Dickey, O.D.Velev “Development of capillary-osmotic wearable patches for sweat analysis of potassium via lateral flow assays”, in-preparation
- T. Saha, S.Mukherjee, M.D.Dickey, O.D.Velev, “Sweat Management in Microfluidic Devices: A Review”, *Lab on a Chip*, under review.
- T.Saha, J. Fang, S.Mukherjee, T.C.Knisely, M.D.Dickey, O.D.Velev “Osmotically Enabled Wearable Patch for Sweat Harvesting and Lactate Quantification” 2021, *Micromachines* 12(12), 1513
- T.Saha, J. Fang, S. Mukherjee, M.D. Dickey, O.D. Velev “A Wearable Osmotic- Capillary Patch for Prolonged Sweat Harvesting and Sensing.” 2021, *ACS Appl. Mater. Interfaces* 13 (7), 8071-8081

- S Mukherjee, S Kumar, R.K. Sahu, S. Nayar “PVA-graphene-hydroxyapatite electrospun fibres as air-filters”, 2019, *Mater. Res. Express*, 6, 125366.
- M.Mahato, S.Mukherjee, T.Mishra “Development of N doped TiO₂ coated Fe₃O₄-SiO₂ nanomaterial as visible light sensitive magnetic photocatalyst for environmental application”, 2019, *Mater. Res. Express*, 6, 105544.
- B.S.Yadav, R.K.Sahu, A.K.Pramanick, T.Mishra, A.Alam, M.Bharati, S. Mukherjee, S.Kumar, S.Nayar. “Collagen functionalized graphene sheets decorated with in situ synthesized nanohydroxyapatite and electrospun into fibers”, 2019, *Mater. Today Commun.*, 18, 167-175.
- S.Mukherjee, V.Parekh, C.T.Puttaswamy. “Design and Fabrication of a Reactor for Alkaline Rich Mineral Waste Carbon Sequestration”, *International Journal of Prevention and Control of Industrial Pollution*, Volume 3, Issue 2, 2017, pp. 1-15.
- S.Mukherjee, V.Parekh, “Review of Purification of Industrial Waste water”, *International Journal of Engineering Research and Technology*, 2016, 5 (8), 379-383.

CONFERENCES

- Oral presentation on “Development of capillary-osmotic wearable patches for sweat analysis of potassium & cortisol via lateral flow assays”, ACS Fall 2021 and ACS Colloids 2022.
- Oral & poster presentation on “Development of capillary-osmotic wearable patches for sweat analysis of potassium & cortisol via lateral flow assays”, Triangle Soft Matter Symposium, Raleigh-Durham, 2021.
- Poster presentation on “Development of capillary-osmotic wearable patches for sweat analysis of potassium & cortisol via lateral flow assays”, Schoenborn & MBTP Research Symposiums, Raleigh, 2021.

TEACHING AND MENTORING

- Teaching assistant for a class of 53 students for Colloids and Interfacial Science (CHE 596) in Spring 2022.
- Teaching assistant for a class of 90 students for Thermodynamics Part 1 and Part 2. (CHE 315 and CHE 316) in Fall 2020 and Spring 2021 respectively.
- Served as a Research Mentor for three Undergraduate students and guided them on different projects

AWARDS AND ACHIEVEMENTS

- Awarded a Mentored Teaching Fellowship (MTF) for the Spring 2022 semester from the College of Engineering for providing teaching assistantship for CHE 596.
- Nominated as one of the five finalists for the Linde Exceptional Teaching Assistant Award in the Department of Chemical and Biomolecular Engineering, NCSU for CHE 316.
- Secured a percentile of 95.3 in the Graduate Aptitude Test Engineering-GATE (March'2016).
- Awarded a stipend-cum-scholarship from the Ministry of Human Resources and Development, Government of India throughout the course of graduate study. (July'16 – May'18)
- Awarded a gold medal and cash prize in the annual convocation for securing a Third rank in the department in undergraduate studies. (July'2017)

VOLUNTEERING EXPERIENCE/EXTRACURRICULARS

- Serving as the Graduate Recruiting Captain for the Department of Chemical & Biomolecular Engineering, NCState for Spring 2022.
- Serving as the Secretary & Webmaster for the Graduate Student Association, CBE, NCState for the year 2021-2022.
- Served as a coordinator for the teams of ‘School Sessions’ and ‘Awareness against Child Sexual Abuse’ for an NGO ‘Child Rights and You’ (CRY) and received a certificate of appreciation from CRY (Kolkata, India, November'16 to May'18).
- Obtained Distinction in Part I of Indian Classical music from Akhil Bharatiya Gandharva Mahavidyalaya Mandal, Mumbai in 2009 and First Division in Senior Diploma Part-II of Art from Sarabharatiya Sangeet-O-Sanskriti Parishad in 2008.

SARVESH ANAND NADKARNI

☎ (984) 683-3337 | ✉ snadkar@ncsu.edu | **in** <https://www.linkedin.com/in/sarvesh-nadkarni/>

EDUCATION

North Carolina State University, Raleigh, NC

Aug. 2022 – May 2024

Masters of Science in Chemical Engineering

- Courses: Chemical Reaction Engineering, Polymer Science, Thermodynamics

Thadomal Shahani Engineering College, University of Mumbai, India

Aug. 2017 – July 2021

Bachelor in Chemical Engineering | **CGPA: 9.12/10**

- Relevant Courses: Heat Transfer Operations, Chemical Reaction Engineering

ACADEMIC ACHIEVEMENTS

- Secured 1st Rank in Chemical Branch in Third Semester with 9.50 CGPA
- Secured 10 CGPA in Chemical Branch in Sixth Semester
- Secured All India Rank (AIR 2) in National Engineering Olympiad

PROJECTS AND INTERNSHIPS

A DETAILED STUDY OF ENERGY STORAGE SYSTEMS | *BE PROJECT*

Aug. 2020 – May 2021

- Compiled core concepts of Energy Storage Systems (ESS) such as its evolution, classification, comparison, current scenario and applications
- Performed efficiency calculations of Pumped Hydro Storage Systems and AA-CAES and compared the result with existing projects
- Examined the environmental impacts and future prospects keeping in mind the ever – growing needs of a developing country, India
- Introduced Gravity-based energy storage as an evolution of pumped hydro storage (PHS) technologies, which can store large quantities of energy using the mass of water at different elevations
- Proposed integration of CAES with renewable energies which can help to improve the overall efficiency of the system

RASHTRIYA CHEMICALS AND FERTILIZERS LIMITED | *INTERN*

Dec. 2019

- Analyzed detailed processes of High Pressure and Medium Pressure Nitric Acid Plant at RCF, MUMBAI
- Examined various raw materials, equipment and maintenance of pump used in the Nitric Acid plant
- Visited Sodium Nitrite/Nitrate plant and studied it during the internship period
- Successfully submitted a detailed report of Nitric Acid plant at end of internship

TECHNICAL TRAINING / CERTIFICATIONS

- Programming for Everybody (Getting started with Python) – Coursera.com
- Excel Skills for Business: Essentials – Coursera.com

TECHNICAL SKILLS

- * **Intermediate:** AutoCAD, MATLAB, Microsoft Excel
- * **Basic:** Python, C

EXPERIENCE

Volunteer of National Service Scheme (NSS-TSEC)

June 2018 – June 2020

Thadomal Shahani Engineering College

Mumbai, India

- * Completed 240 hours of community service under National Service Scheme – Thadomal Shahani Engineering College
- * Arranged various activities like Tree plantation, Blood donation in college and attended a 7-day Residential Camp in adopted village of Neral
- * Attained certificate of appreciation for constructing 30+ Continuous Contour Trenches under Watershed Management program in Neral
- * Volunteered to teach underprivileged students of Neral under Unnat Bharat Abhiyan UBA - TSEC

CO-CURRICULAR ACTIVITIES

- * Organized National Level E-Quizzes on Alternative Energy and Wastewater Management on behalf of Chemical Engineering Department of TSEC
- * Visited Chemtech exhibition 2019 and learned about working of different mechanical equipment used in the Chemical industries
- * Secured 5th rank in School in SSC (10th Standard)
- * Certificate of Appreciation for constructing 30+ Continuous Contour Trenches under Watershed Management program in Neral
- * Participated in 8kms Marathon race to promote Child Rights held in collaboration with CACR

Hwan Oh

401 The Greens Circle, Apt 322, Raleigh, NC 27606
Email: hoh4@ncsu.edu / Cell phone: 984-289-8511

SUMMARY

- A 4th-year Ph.D. candidate in Chemical Engineering Department at NC State University.
- Expected graduation date: May. 20. 2024
- Working on ASD using vapor phase methods (CVD, ALD, and MLD).
- Interned as a thin film engineer at Micron Technology in Summer 2022.
- Looking forward to an internship opportunity in June 2023.

EDUCATION

- Ph.D., Department of Chemical and Biomolecular Engineering** *Aug. 2019 – present*
North Carolina State University, Raleigh, NC
- Advisor: Prof. Gregory Parsons
- M.S., Department of Chemical Engineering** *Mar. 2017 – Feb. 2019*
University of Seoul, Seoul, Korea
- Thesis Title: Next-Generation Flexible Electrochemical Displays: Electrochemiluminescent and Electrochromic Displays
- B.S., Chemical Engineering and Materials Science** *Mar. 2014 – Feb. 2017*
University of Seoul, Seoul, Korea

RESEARCH EXPERIENCE

- Research Assistant, North Carolina State University** *Jan. 2020 – present*
Advisor: Prof. Gregory Parsons
- Area-selective deposition (ASD) of polymers by molecular layer deposition (MLD) or chemical vapor deposition (CVD)
 - Area-selective deposition (ASD) of tungsten and molybdenum by atomic layer deposition (ALD)
 - Research on integration of multiple area-selective deposition (ASD) processes
- Research Assistant, University of Seoul, Korea** *July 2017 – July 2019*
Functional Polymeric Materials Laboratory
Advisor: Prof. Hong Chul Moon
- Research on flexible electrochemical devices based on ion gels; 6 papers published (1st author)

TECHNICAL SKILLS

- **Thin film deposition:** Deposition of organic and inorganic thin films on various substrates using vapor phase methods such as thermal CVD, ALD, and MLD
- **Surface modification:** Surface modification using self-assembly monolayers or inhibitors for ASD
- **Lab techniques:** Ellipsometry, Profilometry, Four-point probe, FTIR, QCM, SEM, AFM, and XPS
- **Data analysis:** OriginLab, MATLAB

PROJECTS

- [1] Orthogonal DoD/MoM Area Selective Deposition for Advanced Nanopatterning, Task ID: 2974.001, July. 1. 2020 ~ Jun. 30. 2023, Semiconductor Research Corporation (SRC)

Awards and HONORS

- Outstanding Paper Award, University of Seoul, Korea (Title: Electrostatic-Force-Assisted Dispensing Printing of Electrochromic Gels for Low-Voltage Displays) (Feb. 2018)
- Outstanding Paper Award, University of Seoul, Korea (Title: Voltage-Tunable Multicolor, Sub-1.5 V, Flexible Electrochromic Devices Based on Ion Gels) (Aug. 2017)

JOURNAL PUBLICATIONS

- [1] **Hwan Oh**, Jae Kyeong, Yong Min Kim, Tae Young Yun, Unyong Jeong*, Hong Chul Moon*, “User-Customized, Multicolor, Transparent Electrochemical Displays Based on Oxidatively Tuned Electrochromic Ion Gels”, *ACS Appl. Mater. Interfaces* **2019**, 11 (49), 45959-45968.
- [2] **Hwan Oh**, Dong Guy Seo, Hong Chul Moon*, “Performance Improvement of Yellow Emitting Electrochemi-luminescence Devices: Effects of Frequency Control and Coreactant Pathway”, *Organic Electronics*, **2019**, 65, 394-400
- [3] Yong Min Kim, Dong Gyu Seo, **Hwan Oh**, Hong Chul Moon*, “A Facile Random Copolymer Strategy to Achieve Highly Conductive Polymer Gel Electrolytes for Electrochemical Electronics”, *Journal of Materials Chemistry C*, **2019**, 7 (1), 161-169
- [4] **Hwan Oh**, Yong Min Kim, Unyong Jeong*, Hong Chul Moon*, “Balancing the Concentrations of Redox Species to Improve Electrochemiluminescence by Tailoring Symmetry of AC Voltage”, *ChemElectroChem*, **2018**, 5, 2836-2841.
- [5] **Hwan Oh**, Dong Gyu Seo, Tae Young Yun, Seong Been Lee, Hong Chul Moon*, “Novel Viologen Derivatives for Electrochromic Ion Gels Showing a Green-Colored State with Improved Stability”, *Organic Electronics*, **2017**, 51, 490-495
- [6] Keon-Woo Kim†, **Hwan Oh**†, Jae Hyun Bae, Haekyoung Kim, Hong Chul Moon*, Se Hyun Kim*, “Electrostatic-Force-Assisted Dispensing Printing of Electrochromic Gels for Low-Voltage Displays”, *ACS Appl. Mater. Interfaces* **2017**, 9 (22), 1899419000. (†equal contribution)
- [7] **Hwan Oh**†, Dong Gyu Seo†, Tae Young Yun, Chan Young Kim, Hong Chul Moon*, “Voltage-Tunable Multicolor, Sub-1.5 V, Flexible Electrochromic Devices Based on Ion Gels”, *ACS Appl. Mater. Interfaces* **2017**, 9 (8), 7658-7665. (†equal contribution)

CONFERENCE PRESENTATION

- [1] **Hwan Oh**, Gregory N. Parsons, Orthogonal DoD/MoM Area Selective Deposition for Advanced Nanopatterning, 2022 Nanomanufacturing Materials and Processes (NMP) Annual Review, in-person event, (Aug. 3 – Aug. 5, 2022, oral presentation)
- [2] **Hwan Oh**, Jung-Sik Kim, Gregory N. Parsons, Dual-Material Area-Selective Depositions for Advanced Nanopatterning: Poly(3,4-ethylenedioxythiophene) (PEDOT) and Tungsten (W) on Si-H/SiO₂ Substrates, 2022 Area-Selective Deposition (ASD) Workshop, in-person event, (Apr. 21 – Apr. 23, 2022, poster presentation)
- [3] **Hwan Oh**, Jung-Sik Kim, Gregory N. Parsons, Sequential Area Selective Deposition of Poly(3,4-ethylenedioxythiophene) (PEDOT) and Tungsten on SiO₂/Si-H Substrates, 21st International Conference on Atomic Layer Deposition, virtual event, (June. 27 – June. 30, 2021, oral presentation)
- [4] **Hwan Oh**, Jung-Sik Kim, Seung Keun Song, Gregory N. Parsons, Orthogonal DoD/MoM Area Selective Deposition for Advanced Nanopatterning, 2021 Nanomanufacturing Materials and Processes (NMP) Annual Review, virtual event, (Mar. 10, 2021, oral presentation)
- [5] **Hwan Oh**, Jung-Sik Kim, Seung Keun Song, Gregory N. Parsons, Orthogonal DoD/MoM Area Selective Deposition for Advanced Nanopatterning, 2020 Nanomanufacturing Materials and Processes (NMP) Kick-Off presentation, virtual event, (Nov. 18, 2020, oral presentation)

REFERENCE

- Prof. Gregory Parsons (Principal investigator)
- Affiliation: North Carolina State University
- E-mail: gnp@ncsu.edu

Kankanige Himendra Perera

khperera@ncsu.edu

(864)-497-2179

EDUCATION

PhD Chemical Engineering, (expected 2024) August 2019-Present
NC State University Raleigh, NC
Experimental and computational rheology 3.85/4.0

B.S. Chemical Engineering May 2019
Clemson University Clemson, SC
Emphasis: Polymers & Applied Engineering, Additional Computer Science Coursework 3.98/4.0

EXPERIENCE

Graduate Researcher January 2020 – Present
Dr. Khan, Chemical Engineering Department, NCSU Raleigh, NC

- Performing rheological studies using AR-2000 and DHR-3 rheometers
- Using ANSYS and OpenFOAM to understand 2-phase viscoelastic flows using computational fluid dynamics
- Utilizing UV-fluorescent confocal microscopy to understand interface between molten polymer streams
- Employing SOLIDWORKS to design extrusion dies and perform stress and temperature analysis to validate die mechanical stability.
- Using OpenFOAM and ANSYS to develop die and die head based on fluid profile for polymer extrusion processes.
- Developing Python code to analyze raw rheology data and perform Fourier-Transform rheology

Undergraduate Researcher January 2017 – May 2019
Dr. Ogale, Center for Advanced Engineering Fibers and Films Clemson, SC

- Characterized polymeric and carbon fiber materials via testing methods including rheology, flexural testing, impact testing, DMA, light microscopy, etc.
- Calibrated and set up new measurement devices for in-depth analysis on unique tests
- Studied the effect of different processing techniques on polymeric materials, such as biaxial stretching or fatigue
- Collaborated with graduate students and professors on a weekly basis for accountability and keeping projects up to date

Research & Development Intern May 2018 – August 2018
Sonoco Products Company Hartsville, SC

- Assigned leadership to two R&D projects in the consumer and industrial packaging areas
- Developed a new testing methodology for determining PET molecular degradation through IR end group analysis
- Analyzed PET compounds via rheology and DSC for performance evaluation.
- Researched and implemented PET vacuum extrusion to reduce hydrolytic degradation in thermoforming process
- Developed prototypes and methodologies for innovative packaging and increased market capability
- *Full time R&D position offered at end of internship as recognition of excellent work*

REU Intern May 2017 – August 2017
Tetramer Technologies Pendleton, SC

- Improved on a fat and calorie reducing modified triglyceride in coordination with Choco Finesse and Blommer
- Characterized biphasic lipid crystal structures through experimental techniques such as DSC, surface energy studies, impact testing, IR spec, polarized light microscopy, and thermocouple-based tests
- Established new testing methodologies and processes based on ASTM standards and theoretical research papers
- Provided suggestions to upper level scientists on new avenues of material application
- Performed statistical analysis on collected data to present conclusions and suggestions to managers for commercial product applications

Creative Inquiry Researcher

August 2016 – December 2016

Dr. Creager – Chemistry Department, Clemson University

Clemson, SC

- Researched scaled down prototype hydrogen fuel cells with a proton exchange membrane
- Pursued unconventional designs to improve fuel cell efficiency and function
- Implemented student originated designs to create innovative fuel cells
- Attended weekly meetings with professors and graduate students to keep track of progress

Research & Development Intern

January 2014 – April 2014

Sealed Air Corporation

Duncan, SC

- Researched the properties of prototyped biodegradable packaging made with renewable resources
- Developed a simple testing method to study, analyze, and evaluate the mechanical properties of the samples
- Statistical analysis of data using Minitab and made conclusions in collaboration with a Senior Scientist
- Final deliverables included a public presentation, graphic panels, and a professional report to company superiors in a roundtable discussion

ADDITIONAL SKILLS

- Computational Fluid Dynamics, Meshing, SOLIDWORKS
- ANSYS and OpenFOAM
- Statistical analysis: including ANOVA, t-tests, and DOE
- Expertise in JAVA, C, C++, Excel, Raspberry Pi, Arduino, and Minitab
- Relevant Coursework: Algorithms & Data Structures, C++, Java

- Python, PANDAS, and Seaborne
- Chemical and polymer synthesis, ATRP, siATRP

Venkat Sashank Punati

vpunati@ncsu.edu | (469) 604-6067 | <https://www.linkedin.com/in/venkat-sashank-punati>

SUMMARY

Passionate and hardworking chemical engineer with profound industrial and laboratory research experience, with expertise in Quantum dot synthesis, flow chemistry and spectroscopy. Other key highlights in work include process operations and design.

EDUCATION

M.Sc., Chemical Engineering

North Carolina State University, Raleigh, NC, USA

August 2021-

GPA:3.8/4.0

B.Tech., Chemical Engineering

National Institute of Technology Raipur, CG, INDIA

August 2016-June 2020

GPA:8.91/10.00

INTERNSHIP

Indian Institute of Chemical Technology, India

November 2020 – March 2021

Hindustan Petroleum Corporation Lt, India

May 2019 – July 2019

PROFESSIONAL EXPERIENCE

Graduate Research Assistant, Department of Chemical and Biomolecular Engineering, North Carolina State University, 2022-Present

- Synthesized Yb Mn doped Cesium Lead Chloride quantum dots by hot injection method along with halide exchange to the cation doping
- Synthesized Lead-free quantum dots by hot injection, to reduce the net lead quantity
- Working on transferring the batch to flow synthesis of quantum dots at high temperature using flow chemistry by microfluidic reactors and automation of the complete system

Dissertation Student, Indian Institute of Chemical Technology, Hyderabad, India, November 2021- March 2022

- Developed a biodegradable transformer oil replacing the current mineral oil.
- Used two-step trans-esterification process for the synthesis of oil
- Compared
- Tested and confirmed the oil using a primitive transformer setup
- The final effective dielectric strength of the sample was 60kV and BDV>40kV

Intern, Hindustan Petroleum Corporation Lt, Visakhapatnam, India, May 2019- July 2019

- Studied in detailed about the operation on gasoline production and intermediate processing units like Fluid Catalytic Cracking and Naphtha Isomerization units

RELEVANT COURSEWORK

- Colloidal Nanoscience and Polymer Rheology
- Reaction Kinetics, Transport Phenomena, Thermodynamics, Process Operations

TECHNICAL SKILLS

Materials Characterization	UV-Vis and PL spectroscopy, GC-MS, TEM, XRD
Experimental Techniques	Flow Chemistry, Organic and Inorganic Materials Synthesis, Cyclic Voltammetry, Esterification
Programming and Software	MATLAB, LabVIEW (basics), Origin, SOLIDWORKS, MS Office

LEADERSHIP ROLES AND ACHIEVEMENTS

- Member of professional development of Chemical & Biomolecular Engineering Graduate Student Association at NC state University
- Secretary in our college as an office bearer for **IICHE Student Chapter** (Indian Institute of Chemical Engineers), NIT Raipur, INDIA
- Secured 1st prize in National wide poster presentation as a part of **Schemcon-2018**, ICT, Mumbai, INDIA by **IICHE**

NANDITA RAAJ KUMAR

Raleigh, NC, USA | (919)-633-0507 | nraajku@ncsu.edu | [My LinkedIn Profile](#)

EDUCATION

North Carolina State University, NC, USA Aug 2021-May 2023

Masters in Chemical Engineering (GPA: **3.67**)

Courses taken in Fall 2022:

- Thermodynamics & Global Regulatory Affairs for Medicine Production

Alagappa College of Technology, Anna University, India

Aug 2016-May 2020

B.Tech. Chemical Engineering

Cgpa: **9.4/10** (Top 5%)

Course Highlights:

- Final year Project – Process design for the Production of Dipentyl ether from n-pentanol
- Petroleum Refining and Petrochemicals, Petroleum Engineering, Industrial Safety Management

RESEARCH AND RELEVANT EXPERIENCE

Axalta Coating Systems LLC, Front Royal VA

May 2022- Aug 2022

Process Technology Intern

- Contributed and worked in the Process Technology and scale-up team responsible for bridging Laboratory testing and manufacturing production of paint batches
- Upgraded and revamped an outdated program from 2002 to maximize the accuracy of adjustment for problematic batches which led to a cycle time reduction of 2 hours per batch
- Revised product formulas for testing and improving manufacturing techniques in TIPSRX software to increase “Right First Time” and production efficiency
- Performed data mining and analysis for over 150,000 viscosity data points to adjust the testing parameters in CAP2000 viscometer saving ~ \$ 10,000
- Created Lab Work Requests (LWRs) in the salesforce which expanded the tax benefits of the company to \$ 4.4 million

Department of Chemical and Biomolecular Engineering, NC State

Jan 2022- Present

Graduate Researcher (Dr. Orlin Velev’s Group)

- Currently working on the capture of microplastics and oil using PLA, PCL, and Polystyrene Soft Dendricolloids (SDCs)

Department of Chemical and Biomolecular Engineering, NC State

Jan 2022- May 2022

Graduate Teaching Assistant

- Worked as a Graduate Teaching Assistant for Green Chemical Engineering
- Organized discussion forums for students to analyze various chemical engineering processes and come up with more environment-friendly and viable methods

Department of Chemical and Biomolecular Engineering, NC State

Aug 2021- Dec 2021

Graduate Teaching Assistant

- Worked as a Graduate Teaching Assistant for Chemical Engineering Design – Undergraduate level
- Conducted office hours to help students with the basics of process simulation in Aspen

Budding Brains Education, India

Jul 2020-Feb 2021

Summer Intern

- Developed flowsheets and simulations in DWSIM software for Natural Gas Plant and production of Industrial chemicals such as Urea, ACN, Dimethyl ether, Cyclohexane, Cumene, Styrene and ETBE
- Prepared and narrated 10 hours of training modules/videos for the above-mentioned Advanced Process simulations

Department of Chemical Engineering, IIT-Madras, India

May-June 2019

Research Intern

- Researched process simulation and Data Reconciliation of a Crude Preheat train
- Simulated flowsheets and Process flow charts in Aspen Plus V10

Project - Bio-ethanol production from lignocellulosic waste

Jan-Mar 2019

Project Assistant

- Synthesized and examined Bio-ethanol production using lignocellulosic waste
- Analysed various Pre-treatment methods of fruit peels

SKILLS

- Lab Experience: Probe Sonicator, DLS, Spectrophotometer, Electron Microscope, gas chromatography, CAP 2000 viscometer, Amine titration, Moisture meter, COMPUTRAC
- Proficient in Expert MS Office (Excel, PowerPoint, Access, Word), Salesforce, TIPSRX, SAP, MATLAB, Aspen Plus, Aspen Hysys, UniSIM Design, DWSIM, MATLAB
- PFD, P&IDs, Control cards and batch cards
- Languages: English, Hindi, Tamil, Kannada, Japanese

Vahid Rahmanian

Phone: 484-655-0700 | E-mail: vrahman@ncsu.edu | linkedin.com/in/vahid-rahmanian

SUMMARY

- Motivated and teamwork-oriented Ph.D. student in chemical engineering with experience in material design, nanofiber synthesis, aerogel fabrication, and rheology.
- Lead of a number of projects over the last 4 years on polymer rheology and aerogel design and fabrication.
- A quick learner with teamwork skills and enthusiastic about research.

EDUCATION

North Carolina State University <i>Ph.D. in Chemical Engineering, GPA: 4/4</i>	Raleigh, NC, USA <i>Aug. 2018 – Present</i>
Lehigh University <i>M.Sc. in Chemical Engineering, GPA: 3.57/4</i>	Bethlehem, PA, USA <i>Aug. 2016 – May 2018</i>
Sharif University of Technology <i>M.Sc. in Polymer Engineering, GPA: 3.89/4</i>	Tehran, Tehran, Iran <i>Aug. 2012 – Jan. 2015</i>
Iran University of Science and Technology <i>B.Sc. in Chemical Engineering, GPA: 3.98/4</i>	Tehran, Tehran, Iran <i>Aug. 2008 – Jul. 2012</i>

SKILLS

Experimental and Analytical Skills: Material synthesis and characterization; Electrospinning hybrid nanofibers; Nanofibrous aerogel design; Polymer and hydrogel rheology; Rheology of powder coatings; High pressure rheology; FTIR spectroscopy; Electron microscopy and EDS analysis; UV-Vis spectroscopy; TGA, DCS, XPS and XRD analysis
Computational Skills: MATLAB, Aspen Plus, Mathematica, Origin, LaTeX, C, C++
Professional Skills: Leadership, Problem-solving, Project and task management, Collaboration and teamwork

LEADERSHIP

Powder coating rheology: This was an industrial project in collaboration with Eastman Chemical Company in which I led the NC State team, consists of two Ph.D. and one master students, to investigate the curing behavior and perform fundamental characterization of powder coating formulation to address the surface defect formation.
High pressure rheology: This is a current project in collaboration with Eastman Chemical Company. In this project, I am leading the NC State team, consists of two Ph.D., one masters, and one undergraduate students to investigate the ability of using plasticizer (i.e., CO₂, n-pentane and iso-pentane) to enhance production or reduce processing temperature of cellulose esters.

SELECTED PUBLICATIONS AND CONFERENCES

- **V. Rahmanian**, T. Pirzada, S. Wang, and S. A. Khan, 2021. Cellulose-Based Hybrid Aerogels: Strategies Towards Design and Functionality, *Advanced Materials*, 33(51) p.2102892.
- T. Pirzada, **V. Rahmanian**, and S. A. Khan, (2021) Nanofiber Aerogels: Bringing Third Dimension to the Electrospun Nanofibers in A. L. Andrady, and S. A. Khan (1st) *Applications of Polymer Nanofibers*. John Wiley and Sons. Chapter 9, page 347-373.
- Janke, A.M., Seo, D.H., **Rahmanian, V.**, Conicella, A.E., Mathews, K.L., Burke, K.A., Mittal, J. and Fawzi, N.L., 2017. Lysines in the RNA Polymerase II C-Terminal Domain Contribute to TAF15 Fibril Recruitment. *Biochemistry*, 57(17), pp.2549-2563.
- Hasany, M., Malakootikhah, M., **Rahmanian, V.** and Yaghmaei, S., 2015. Effect of hydrogen combustion reaction on the dehydrogenation of ethane in a fixed-bed catalytic membrane reactor. *Chinese Journal of Chemical Engineering*, 23(8), pp.1316-1325.
- **Vahid Rahmanian**, Tahira Pirzada, Eduardo Barbieri, Saad A. Khan. "Photo-Responsive aerogel designed from sol-gel electrospun PVP-TiO₂ nanofibers." 2022 ACS Spring Meeting, San Diego, CA.
- **Vahid Rahmanian**, Young C. Kim, Jeetain Mittal. "Multicomplex Formation in the Presence of Polymer Crowders Mimicking in-Cell Environment." 2017 AIChE Annual Meeting, Minneapolis, MN.

PROJECTS

Design of Aerogels from Electrospun Nanofibers

Nov. 2018 – Present

- Design, synthesis and characterization of hybrid nanofibrous aerogels (NFAs). Investigate the interaction of components and their effect on the properties and functionality of NFA.
- Investigate post-processing approaches (i.e. chemical crosslinking, thermal treatment, surface modification) and integrating functional materials to impart new functionality and desirable physical properties to the NFAs.

High pressure rheology of cellulose esters

Sponsored by Eastman Chemical Company

Aug. 2021 – Present

- Investigate use of plasticizers in an effective way to enhance processing performance of cellulose esters.
- Conduct rheological experiments at different temperature and pressure to develop a fundamental baseline on the effect of plasticizers (i.e., CO₂, n-pentane and iso-pentane) on cellulose esters.
- Collaborated in a group of 8 individuals, both at Eastman Chemical Company and NC State University, toward a common goal to address cellulose ester processing issues using high pressure rheology as a tool.

Rheological and Structural Analysis of Thermosetting Powder Coatings

Sponsored by Eastman Chemical Company

Aug. 2019 – Jul. 2020

- Fundamental characterization of powder coating formulations towards understanding surface defect formation.
- Perform rheological experiments to investigate the curing behaviour of powder coatings.
- Collaborated in a group of 7 individuals, both at Eastman Chemical Company and NC State University, toward a common goal which resulted in a baseline understanding on surface defect formation and a journal article.

Molecular Dynamic Simulation

Nov. 2016 – May 2018

- Investigated binding interaction between higher order assembly of FET (FUS, EWSR1 and TAF15) low complexity domain oncoproteins with C-terminal domain of RNA polymerase II using all-atom simulation method.
- Studied the macromolecular crowding effects on the diffusion and kinetics of binding interaction of Ubiquitin/UIM1 complex in the presence of polymeric crowders mimicking in-cell environment using coarse-grained model.

EXPERIENCE

Research Assistant

North Carolina State University

Nov. 2018 – Present

- Design, synthesis, and characterization of multifunctional nanofibrous aerogels
- Leading projects on rheological and structural analysis of powder coating formulations
- Effect of plasticizers on cellulose ester using high pressure rheology technique to enhance production efficiency

Lehigh University

Nov. 2016 – May 2018

- Performing all-atom simulation on binding interaction of intrinsically disordered proteins
- Performing coarse-grained simulation to understand the kinetics of binding interaction of Ubiquitin/UIM1 complex in the presence of polymeric crowders mimicking in-cell environment

Teaching Assistant

North Carolina State University

Jan. 2019 – Dec. 2021

- Polymer Rheology (CHE 596) by Dr. Saad A. Khan (Summer 2020, Spring and Summer 2021)
- Transport Phenomena II (CHE 312) by Dr. Milad Abolhassani and Dr. Saad A. Khan (Spring 2019, Spring 2020)
- Chemical Engineering Laboratory (CHE 330) by Dr. Hassan Golpour (Fall 2019, Fall 2021)

Lehigh University

Aug. 2017 – May 2018

- Methods of Analysis in Chemical Engineering (CHE 201) by Dr. Mark Snyder (Fall 2017)
- Chemical Engineering Fundamentals III (CHE 383) by Dr. Cesar Silebi (Spring 2018)

HONORS AND AWARDS

- Linde exceptional teaching assistant award, 2020, awarded by CBE Department at NC State University
- Graduate merit award, 2018, awarded by College of Engineering at NC State University
- Lehigh presidential fellowship, 2016, Offered upon the recommendation of the faculty of Lehigh University
- Ranked 1st, class of 2015, Chemical Engineering Department, Sharif University of Technology
- Ranked 1st, class of 2012, Chemical Engineering Department, Iran University of Science and Technology

VOLUNTEER JOBS

- **Volunteer Organizer** at Society of Rheology conference, Raleigh Conventional Center, NC, October 2019
- **Instructor** at Persian School at Iranian Cultural Society of North Carolina, 2019 – 2020
- **Communication Officer** of Lehigh University Iranian Students Association, 2017 – 2018

Prattasha Sarker

625 Centennial Parkway, Apt 104, Raleigh, 27606 Tel: (336)-661-7754
Email: prattasha140@gmail.com | LinkedIn: [prattasha-sarker-94a535147](https://www.linkedin.com/in/prattasha-sarker-94a535147)

EDUCATION

North Carolina State University <i>Doctor of Philosophy in Chemical and Biomolecular Engineering; GPA: 3.93/4.0</i>	Raleigh, North Carolina Aug 2019-Expected Graduation Jul 2024
North Carolina State University <i>Master of Science in Chemical and Biomolecular Engineering; GPA: 3.93/4.0</i>	Raleigh, North Carolina Aug 2019-Dec 2021
Bangladesh University of Engineering and Technology <i>Bachelor of Science in Chemical Engineering; GPA: 3.92/4.0</i>	Dhaka, Bangladesh Jul 2014 - Oct 2018

AREA OF EXPERTISE

-
- | | | |
|------------------------------------|------------------------------|--------------------------------|
| • Rheology | • Live dead assay/ MTT assay | • Dynamic Mechanical Analysis |
| • Tissue Regeneration | • Confocal Imaging | • Thermogravimetric Analysis |
| • Biomaterials Engineering | • UV-Vis Spectroscopy | • Scanning Election Microscopy |
| • Isothermal Titration Calorimetry | • FTIR spectroscopy | • ASPEN HYSYS/ Origin/ MATLAB |

EXPERIENCE AND NOTABLE CONTRIBUTIONS

North Carolina State University <i>Graduate Research Assistant</i>	Raleigh, NC Aug 2019 - Present
<ul style="list-style-type: none">◦ Advisor: Dr. Saad A Khan◦ Research focus:Applying rheological measurement techniques to bio-based injectable hydrogel in tissue regeneration◦ The overarching goals of the current projects are to examine the following material platform:<ul style="list-style-type: none">* Injectable bio-based hydrogels of collagen and ECM-based materials* Morphology-controlled tannic acid particles incorporated in collagen and ECM-based hydrogels* Cellulose nanofibrils combined with collagen and ECM-based materials* Within each system, the critical issues to be addressed include but not limited to:<ul style="list-style-type: none">* Inquire how the injectability of pre-gel solution, gelation kinetics, final gel stiffness and yielding behavior of the collagen and ECM-based hydrogels get altered by controlling their concentrations, digestion conditions and thermal environments through rheological studies.* Explore the role of biodegradable morphology-controlled tannic acid particles on improving the mechanical properties of bio-based hydrogels.* Investigate how interpenetrating polymer networking can enhance the overall hydrogel strength and stiffness by integrating nature-derived cellulose nanofibrils into the injectable hydrogels.	
North Carolina State University <i>Graduate Teaching Assistant</i>	Raleigh, NC Aug 2020 - Present
<ul style="list-style-type: none">◦ Served as a TA for CHE 311H, Transport Processes I Honors (Fall 2020), CHE 715, Fundamentals of Transport Phenomena (Spring 2021, Summer 2021)◦ Currently serving as a TA for CHE 311H, Transport Processes I Honors (Fall 2022)◦ Taught two lectures for CHE 311H Transport Processes I Honors (Fall 2022)◦ Held weekly office hours and graded homework, quizzes, and exams	
Bangladesh University of Engineering and Technology <i>Undergraduate Researcher</i>	Dhaka, Bangladesh Mar 2016 - Oct 2018
<ul style="list-style-type: none">◦ Advisor: Dr. Syeda Sultana Razia and Md. Ahaduzzaman Nahid◦ Research focus:Chemical Disposal System and Data Analysis on Major Industries of Bangladesh◦ Thesis: Development of low-cost antibacterial paper for health, food and water filtration application◦ Advisor: Dr. Mohidus Samad Khan◦ Focus: The main focuses of selected thesis project are:<ul style="list-style-type: none">* Coating antibacterial agents (quaternary ammonium salts, metal oxide nanoparticles, etc.) on paper surface.* Finding the efficacy of the paper coated with antibacterial agents in reducing the number of bacteria through qualitative and quantitative analysis.* Have been working on finding minimum inhibitory concentration (MIC) of antibacterial agents based on their individual toxicity level	

ARTICLES

- Prottasha Sarker, Danielle M. Nalband, Donald O. Freytes, Orlando J. Rojas and Saad A. Khan, 'High Axial Aspect Tannic Acid Microparticles Facilitates Gelation and Injectability of Collagen-based Hydrogels, *Biomacromolecules*, 2022
- Camilo Mora-Navarro, Mario Eduardo Garcia, Prottasha Sarker, Emily W Ozpinar, Jeffrey Enders, Saad Khan, Ryan Branski, Donald O Freytes 'Monitoring decellularization via absorbance spectroscopy during the derivation of extracellular matrix scaffolds', *Biomedical Materials*, vol. 17, no. 1, Nov 2021
- Ahaduzzaman, Prottasha Sarker, Aniq Anjum and Easir A Khan 'Overview of Major Industries in Bangladesh,' *Journal of Chemical Engineering*, vol. 30, no. 1, pp. 51–58, Dec 2017.

PRESENTATIONS

- Going to present poster on "Rheology of collagen-based hydrogels tailored by tannic acid particles" in Fall Schoenborn Graduate Research Symposium on October 31,2022 at NC State
- Going to attend the 93rd Annual Meeting of The Society of Rheology at Chicago, Illinois from October 9-13,2022 and going to have an Oral Presentation on Tuning the Rheology of Collagen-based Hydrogels using Tannic Acid Particles
- Attended 96th ACS Colloids and Surface Science Symposium at Golden, Colorado from July 10-13, 2022, and had an Oral Presentation on "Rheology of collagen-based hydrogels tailored by tannic acid particles"
- Presented Poster on "Modulating the Rheology of Collagen-based Hydrogels using Tannic acid Particles" in Triangle Soft Matter Workshop on May 9,2022 at Duke University
- Presented Poster on "Modulating the Rheology of Collagen-based Hydrogels using Morphology-controlled Tannic acid Particles" in 2021 Fall Schoenborn Graduate Research Symposium on September 28,2021 at McKimmon Conference Center at NC State
- Attended the 92nd Annual SoR Meeting in-person at Bangor, Maine from October 10-14,2021 and presented poster on Collagen-Tannic acid-based hydrogels
- Attended the Annual Paper Meet- 2017, Chemical Engineering Division, The Institute of Engineers, Ramna, Dhaka-1000, Bangladesh, Oct 2017
- Presented poster on 'Zero Discharge Effluent Treatment Plant' in Fifth International Conference on Chemical Engineering: ICChE, Dhaka, Bangladesh, Dec 2017

AWARDS & ACHIEVEMENTS

- Provost Doctoral Fellowship, fall 2019 through fall 2020, North Carolina State University
- 3rd prize winner in Poster Competition, 2021 Fall Schoenborn Graduate Research Symposium on September 28 at McKimmon Conference Center at NC State
- Dean's List, fall 2014 through fall 2018, BUET for attaining CGPA of 3.75 or higher in two consecutive terms
- University Merit Scholarship, fall 2014 through fall 2018, BUET which is awarded for notable achievement after completion of an academic term
- Champion at Poster Competition, June 2016 issued by Department of Chemical Engineering BUET

Sudeep Sarma

919.785.6981 | ssarma2@ncsu.edu | [LinkedIn](#) | [Research Webpage](#) | [Google Scholar](#)

SUMMARY

Creative, collaborative, and enthusiastic, I am a computational biophysicist and chemical engineer by training who is passionate about fundamental and applied research in protein design and aggregation and molecular biology and aspires to solve complex problems in human healthcare using quantitative methods. I enjoy discussing science and technology with the public and scientists alike.

EDUCATION

- Ph. D, North Carolina State University, GPA – 4.0/4.0** May 2020-2023 (Expected)
Chemical and Biomolecular Engineering, Minor in Biomanufacturing
Advisor: Carol K. Hall
- M.S, North Carolina State University, GPA – 3.978/4.0** Aug 2018-April 2020
Chemical and Biomolecular Engineering
Advisor: Carol K. Hall
- B.S, Malaviya National Institute of Technology (NIT Jaipur), GPA-8.39/10.0** Aug 2014-May 2018
Chemical Engineering
-

RESEARCH INTERESTS

- Computational protein-binder design
 - Protein-protein and peptide-protein interactions, and protein aggregation
 - Computational design of peptide-based biomaterials
 - Molecular simulation techniques, Monte-Carlo methods, optimization techniques and machine learning
-

PROFESSIONAL EXPERIENCE

North Carolina State University | Graduate Research Assistant with Dr. Carol Hall | Raleigh, USA Oct. 2018-Present
Computational peptide design to discover high affinity peptide binders and self-assembling biomaterials

- Designed peptide inhibitors that bind to *Clostridium difficile* toxins via a Monte Carlo (MC) based search algorithm and molecular-level simulations, that block toxin-derived toxicity in small intestinal and large intestinal cells. Filed an Invention Disclosure based on this work.
- Designed peptide inhibitors via an MC based search algorithm and molecular-level simulations that bind to SARS-CoV-2 virus and prevent cellular entry of SARS-CoV-2 virus.
- Designed peptide inhibitors via an MC based search algorithm and molecular-level simulations that binds to MHC Class 1 H-2K^b protein and prevents nonalcoholic steatohepatitis (NASH) progression in mice models.
- Developed a Monte-Carlo search algorithm in fortran90 to design peptides that self-assemble to form amyloid-like structures.
- Performed quantum chemistry calculations to derive partial charges of organic molecules using Gaussian and AMBER.
- Conducted, and managed highly parallelized molecular simulations on local and national computing clusters using Linux/Unix systems.
- Wrote bash scripts and user-friendly code in Fortran90, R and Python to perform molecular simulations, automate workflows and analyze large data sets of simulation trajectories.
- Communicated and presented research projects in reviewed journal articles, international conferences, and external collaborators

Roivant Sciences (Immunovant) | Process Development and Technology Operations Intern | Durham May 2019-December 2019

- Created master datafiles and process flow diagrams of upstream, downstream, analytical development and drug product data for RVT-1401, a monoclonal antibody targeting autoimmune disease; visualized process variability by graphing control charts and calculated Key Performance Indicators (KPIs).
- Reviewed master batch process records prior to Phase III Clinical Trial manufacturing by validating against SOPs and Process Control Strategy documents.
- Performed statistical analysis of tech transfer runs between different Contract Manufacturing Organizations (CMOs) and Design of Experiment (DOE) runs to optimize process parameters for cGMP manufacturing of drug substance.
- Tracked and organized CMC purchase orders, budget allocations, generated timelines, and Gantt Charts for CMC activities, and maintained records of shipment and storage of drug substance and drug product.
- Performed multivariate data analysis, hypothesis testing and ANOVA for FACS and ELISA assay validation.
- Assisted in writing CMC section of IND/IMPd and authored change control documents for tech transfer and internal quality and CAPA management.

University of Saskatchewan | Summer Research Intern with Dr. Christine Soteros, Saskatoon, Canada June 2017 – July 2017
Monte-Carlo simulations to compute probability of DNA Knotting

- Conducted and managed Monte Carlo simulations in the Westgrid Computing Cluster of Canada.
- Used a Markov Chain Monte Carlo algorithm known as the Pivot Algorithm written in C to obtain knot probabilities of DNA and compared the stochastic simulation results with experimental results.
- Optimized parameters of the stochastic algorithm by using an adaptive Robbins Monro mathematical technique.
- Wrote user friendly code in MATLAB to analyze simulation results and optimize the simulation parameters.

AWARDS AND RECOGNITION

- Early Career Researcher Award** | National Science Foundation August 2022
- Awarded the Early Career Researcher Award by the National Science Foundation (NSF) to attend FOMMS (Foundations of Molecular Modeling and Simulation) 2022 held in Delavan, Wisconsin.
- Graduate Student Travel Assistance Award** | NC State University Graduate School August 2022
- Awarded the Graduate Student Travel Awarded by the NC State University Graduate School to attend FOMMS (Foundations of Molecular Modeling and Simulation) 2022 held in Delavan, Wisconsin.
- Mentored Teaching Fellowship** | NC State University August 2021-December 2022
- Awarded for teaching graduate Transport Phenomena
 - The goal of the MTA Program is to provide engineering graduate students with an opportunity to gain teaching experience beyond that of a regular teaching assistant prior to entering an academic career.
- Graduate Merit Award** | NC State University August 2020-May 2021
- This award is provided through funds from the College of Engineering. It is awarded to a small number of outstanding graduate students and top applicants to the graduate program.
- Finalist of Linde Exceptional Teaching Assistant Award** | NC State University Spring'20 and Spring'21
- Nominated in Spring'20 and Spring'21 for teaching graduate Transport Phenomena
 - The award recognizes the instructional effectiveness and class management of Ph.D. candidates serving as exemplary teaching assistants (TAs) in the Chemical Engineering Department.
- 2nd Runner Up Poster Award, Schoenborn Graduate Research Symposium 2020** | NC State University September 2020
- Poster title: "*In-Silico* Discovery of Target Peptide Inhibitors for *C. diff.* Toxins A and B
- Summer Undergraduate Research Internship Award** | Malaviya National Institute of Technology Jaipur May 2017
- Awarded fellowship for research exchange at the University of Saskatchewan

LEADERSHIP EXPERIENCE

- Professional Development Chair | CBE Graduate Student Association | NC State University June 2020-May 2021
- Planned and organized professional development events for graduate students in the chemical engineering department.
 - Facilitated student-alumni conversations and relationships through seminars and talks.
- NC State Entrepreneurship Ambassador | NC State University June 2021-Present
- Support communications and public relations for NC State Entrepreneurship by recruiting, informing, and engaging students throughout the campus.
 - Represent NC State Entrepreneurship at events for outside the NC State community.
- Institute Lawn Tennis Captain | Malaviya National Institute of Technology Jaipur 2016-2018
- Played competitive tennis and represented the college tennis team at national level competitions

PUBLICATIONS (* Equal contribution)

- X. Xiao*, A. S. Robang*, **S. Sarma***, A. K. Paravastu, C. K. Hall. "Sequence Patterns and Signatures: Computational and Experimental Discovery of Amyloid-Forming Peptides", *PNAS Nexus*, *under review*.
- S. Sarma***, S. M. Herrera*, X. Xiao, G.A. Hudalla, C.K. Hall. "Computational Design and Experimental Validation of ACE2-derived Peptides as SARS-COVID 2 Receptor Binding Domain Inhibitors", *J. Phys. Chem. B* **2022**, DOI: [10.1021/acs.jpcc.2c03918](https://doi.org/10.1021/acs.jpcc.2c03918).
- X. Xiao*, R. Kilgore*, **S. Sarma**, S. Menegatti, C. K. Hall. "De novo Discovery of Peptide-based Affinity Ligands for the Fab Fragment of Human Immunoglobulin G", *J. Chromatogr. A* **2022**, DOI: [10.1016/j.chroma.2022.462941](https://doi.org/10.1016/j.chroma.2022.462941).
- X. Xiao, **S. Sarma**, S. Menegatti, N. Crook, S. T. Magness, C. K. Hall. "In-silico Identification and Experimental Validation of Peptide-Based Inhibitors Targeting *Clostridium difficile* Toxin A", *ACS Chem. Biol.* **2022**, DOI: [10.1021/acscchembio.1c00743](https://doi.org/10.1021/acscchembio.1c00743)

ORAL PRESENTATIONS (Selected)

- S. Sarma**, X. Xiao, S. Menegatti, N. Crook, S. T. Magness, C.K. Hall. "*In silico* discovery of target peptide inhibitors for *C. diff* Toxin A and B", *2021 AIChE Annual Meeting*; November 7-19; Session: Data-Driven Design and Modeling I.
- S. Sarma**, X. Xiao, S. Menegatti, N. Crook, S. T. Magness, C.K. Hall. "*In silico* discovery of target peptide inhibitors for *C. diff* Toxin A and B", *2020 Virtual AIChE Annual Meeting*; November 16-20; Session: Protein and Immunoengineering for Human Health.

POSTER PRESENTATIONS

- S. Sarma**, S. M. Herrera, X. Xiao, G.A. Hudalla, C.K. Hall. "Computational Design and Experimental Validation of ACE2-derived Peptides as SARS-COV-2 Receptor Binding Domain Inhibitors", Poster presented at: *2022 FOMMS (Foundations of Molecular Modeling and Simulation)*
- S. Sarma**, X. Xiao, S. Menegatti, N. Crook, S. T. Magness, C.K. Hall. "*In silico* discovery of target peptide inhibitors for *C. diff* Toxin A and B", Poster presented at: *ACS Spring 2021*; April 21; Division of Biological Chemistry.
- S. Sarma**, X. Xiao, S. Menegatti, N. Crook, S. T. Magness, C.K. Hall. "*In silico* discovery of target peptide inhibitors for *C. diff* Toxin A and B", Poster presented at: *Schoenborn Graduate Research Symposium*; 2020 September 22; North Carolina State University, Raleigh, NC (3rd Place Poster Session winner).

SREE RATNA SAMEERA VELLORE

Raleigh, NC, USA | 858.354.4344 | svellor2@ncsu.edu | <https://www.linkedin.com/in/sameera-vellore-7511641b3/>

EDUCATION

North Carolina State University, Raleigh, NC, USA May 2023

Masters in Chemical Engineering | CGPA: 3.55/4

Courses: Chemical Process Modeling, Chemical Reaction Engineering, Polymer Science and Technology, Transport Phenomena, Colloid Science and Nanoscale Engineering, Thermodynamics

National Institute of Technology Raipur, India May 2020

Bachelor of Technology in Chemical Engineering | GPA: 8.61/10

Course Highlights:

- Major project on “Synthesis of Silver Nanoparticles from silver nitrate using leaf extracts”. (2020)
-

RESEARCH AND RELEVANT EXPERIENCE

Department of Chemical and Biomolecular Engineering, Velev Group, NC State Aug 2021-Present

- Thesis research in Dr. Velev’s lab group on the project “Visualization of Fluorescent dyed virus and Virus Like Particles” in collaboration with Unilever.
- DLS analysis and fluorescent microscopy are used for characterization and studies to detect and visualize nanoparticles.

Department of Chemical and Biomolecular Engineering, NC State

Graduate Grading Assistant

Aug 2021- Present

- Assist the faculty through the course by grading the assignments and exams.

Graduate Teaching assistant

May-June 2022

- Assisted students in taking the course “Energy/Material balances” by conducting tutorials and clearing their doubts.

CSIR-IICT [Hyderabad, India] 2019, 2020-2021

Summer Intern (May - June 2019) | Research Project with a scientist (Nov 2020-March 2021)

- Project Assistant for research on “Extractive distillation of ethyl acetate-ethanol-water ternary system using deep eutectic solvent (DES): A techno economic and energy assessment” and paper published. <https://doi.org/10.1016/j.cep.2022.108913>
- Synthesized the DES, used a lab-scale distillation setup and Gas Chromatography Mass Spectroscopy (GCMS) to assess the separation of the ternary mixture of Ethyl Acetate, Ethanol and Water.
- Project assistant for research on “Membrane separation of a Binary mixture using pervaporation” where I analyzed the separation of Ethanol and water using a Membrane pervaporation setup.

Nuclear Fuel Complex, [Hyderabad, India] May-June 2018

- Received 4-weeks industrial training at Nuclear Fuel Complex (NFC) in Zirconium oxide plant in Hyderabad
 - Comprehended the plant design, operations and equipment.
-

ADDITIONAL PROJECT EXPERIENCE

- Synthesized silver nanoparticles with an environmentally benign procedure and characterized using EDAX and SEM analysis. (2019)
 - Experimented and presented on “Equilibrium studies of citric acid with different diluents” for SCHEMCON 2018 and was awarded 2nd place in Oral presentation for the same.
-

LEADERSHIP EXPERIENCE & SKILLS

- Member of IICHE student body of NIT Raipur 2018 - 2020
 - **Software:** MS Office, Basics in C, C++, Aspen Plus, MATLAB, Origin
 - Additional Conceptual skills - Plant design, Fluid mechanics, Process Equipment Design and Dynamics,
 - Coordinator in Shaurya, Sports committee of NIT Raipur, SAMAR 2018 organizing team.
 - Captain, NIT Raipur Basketball team
-

Alison C. Waldman

(862) 812-2294 || acwaldma@ncsu.edu || <https://www.linkedin.com/in/alison-cristine-waldman/>

EDUCATION

North Carolina State University – Raleigh, NC	2018-present
PhD Candidate, Chemical Engineering, <i>Biomolecular Engineering w Biotechnology and Biomanufacturing focuses</i>	
· GPA 3.56/4.0	
M.S. Chemical Engineering	May 2021
Virginia Tech (VT) – Blacksburg, VA	
B.S. Biological Systems Engineering, Honors College	
· Minors: Biomedical Engineering, Green Engineering, Chemistry	
· GPA 3.84/4.0 (In-Major 3.95), Summa Cum Laude graduate and Honors Scholar	

PUBLICATIONS

-
- Waldman, A. C.**, Rao, B. M., & Keung, A. J. (2021). Mapping the residue specificities of epigenome enzymes by yeast surface display. *Cell Chemical Biology*, 28. <https://doi.org/10.1016/j.chembiol.2021.05.022>
- Saylor, K., **Waldman, A.**, Gillam, F., & Zhang, C. (2020). Multi-epitope insert modulates solubility-based and chromatographic purification of human papilloma virus 16 L1-based vaccine without inhibiting virus-like particle assembly. *Journal of Chromatography A*, 1631, 461567. <https://doi.org/10.1016/j.chroma.2020.461567>

PRESENTATIONS

-
- Waldman, A., Keung, A.J., Rao, B.M. "REMY: A rapid and facile method to map the specificities of epigenomic enzymes", ACS Spring National Meeting, New Technologies in Protein Engineering. **Accepted, Oral Presentation.** March 2022.
- Waldman, A. "Mapping the Residue Specificities of Epigenome Enzymes by Yeast Surface Display" Genetics and Genomics Initiative Retreat, **Paper of the Year, Oral Presentation.** Raleigh, NC. August 2021.
- Waldman, A. "Using Yeast Surface Display to Study Epigenomic Enzymes" Genetics and Genomics Initiative Flask Talks. Raleigh, NC. August 2021.
- Waldman, A., Keung, A.J., Rao, B.M. "Mapping the residue specificities of epigenomic enzymes using yeast surface display", NCSU Molecular Biology Training Program Student Symposium, Poster. Raleigh, NC. Nov 2021
- Waldman, A., Keung, A.J., Rao, B.M. "A yeast surface display platform to profile and engineer epigenome editors", NCSU Molecular Biology Training Program Student Symposium, Poster. Raleigh, NC. Oct 2020
- Waldman, A., Keung, A.J., Rao, B.M. "A facile platform for the rapid profiling and engineering of epigenome editors". NCSU CBE Schoenborn Research Symposium, Poster. Raleigh, NC. Jan 2020

PROFESSIONAL EXPERIENCES

Gene Therapy Co-op , <i>Biogen, Cambridge MA</i>	2022-present
Gene Therapy Cell Line Technologies and Proteins Cell Line Development groups	
Graduate Research and Teaching Assistant , <i>NC State University</i>	2019-present
Chemical and Biomolecular Engineering Department, Dr. Albert J. Keung, Dr. Balaji M. Rao	
· Developed a High Throughput Platform to Map the Residue Specificities of Histone Acetyltransferases	
· Managing two undergraduate researchers conducting independent research projects	
· yeast surface display, protein engineering, flow cytometry, molecular biology cloning, experimental design and troubleshooting	
· completed coursework in protein interactions, viral biotechnology, downstream processing, and bioreactor design	
Undergraduate Research Assistant , <i>Virginia Tech</i>	2016-2018
Biological Systems Engineering Department, Dr. Mike Zhang	
· Conducted vaccine delivery and organ collection from laboratory mice	
· Trained in an assay for production of PLGA nanoparticles for drug delivery use	
Biomedical Engineering Intern , <i>Carilion Roanoke Memorial Hospital</i>	2017
Virginia Tech-Carilion Clinic, Mark Skelton and Dr. Jake Soccha	
· Shadowed biomedical engineers and physicians in various hospital departments	

Alison C. Waldman

(862) 812-2294 || acwaldma@ncsu.edu || <https://www.linkedin.com/in/alison-cristine-waldman/>

- NSF REU Intern**, Center for the Environmental Implications of NanoTechnology (CEINT) 2016
Pratt School of Engineering, Duke University, Dr. Emily Bernhardt and Dr. Marie Simonin
· Contributed to Simonin et. al. *Plant and Microbial Responses to Repeated Cu(OH)₂ Nanopesticide Exposures Under Different Fertilization Levels in an Agro-Ecosystem*.
Frontiers in Microbiology, 2018.
- Undergraduate Research Assistant**, *University of South Carolina* 2015
Environmental Analytical Chemistry, Dr. Susan D. Richardson, mentor
· Conducted chlorine and chloramine testing on waters in Columbia, SC

LEADERSHIP AND OUTREACH ROLES

- Engineering Biology, NSF EFRI REM, NC State** 2021
· Team Lead for a group of underrepresented high school students, college students, and community members interested in STEM careers
- Student Leadership and Engagement, NC State** 2019-present
· Student Engagement Intern 2021-present
· Leadership and Civic Engagement Ambassador 2019-2021
· Leadership Development Program, participant 2019, facilitator and coach 2020-present
- Graduate Student Association, NC State** 2019-2022
· 2022 Graduate Recruitment Captain
· 2019-2021 Vice President of External Affairs for Chemical and Biomolecular Engineering
· 2019-2021 University Community and Social Engagement Committee
· 2021 Science House at NCSU, day camp volunteer 2015-2018
- Alpha Omega Epsilon Sorority, Virginia Tech** 2016-2018
· Executive Board, Secretary 2017-2018 academic year
- Society of Agricultural and Biological Engineers (ASABE), Virginia Tech** 2014-2018
· Chapter Secretary, 2016-2018, awarded best chapter in the Southeastern region, 2016-2017
- Center for the Enhancement of Engineering Diversity (CEED), Virginia Tech**
· CEED STEM summer camps assistant 2018
· Women's Preview Weekend Planning Committee 2015-2017
· Hypatia Living Learning Community, Service Learning Committee member 2015-2016

AWARDS AND HONORS

- NC State CBE Vivian T. Stannett Award for Outstanding Early Publication, Runner Up 2022
- NC State Genetics and Genomics Academy, Travel Award 2022
- NC State Genetics and Genomics Initiative, Paper of the Year 2021
- Named NCSU Dean's Doctoral Fellow 2018
- Phi Beta Kappa Honor Society 2018
- Named VT College of Engineering McAllister Leadership Scholar 2017
- Alpha Epsilon, Biological Engineering Honor Society 2017
- The Order of Omega, Greek-life Honor Society 2017
- Phi Kappa Phi Honor Society 2016
- Tau Beta Pi, Engineering Honor Society 2015

Daniel James Willard

601 Rookwood Court
Wake Forest, NC 27587

djwillar@ncsu.edu
(724) 766-9334

Education	North Carolina State University , Raleigh, NC PhD Candidate Minor in Biotechnology Cumulative GPA: 4.00/4.00 Master of Science in Chemical Engineering	August 2018 – Present Received Fall 2020
	Bucknell University , Lewisburg, PA Bachelor of Science in Engineering Major: Chemical Engineering, Concentration: Materials Science Cumulative GPA: 3.77/4.00; Engineering GPA: 3.90/4.00 Dean's List all academic semesters	Graduated May 2015
	University of Queensland , St. Lucia, QLD, Australia Study Abroad during first semester of Junior year	July, 2013 – November 2013

Professional Experience

<i>PhD Candidate</i> , Kelly Hyperthermophiles Group at North Carolina State University , Raleigh, NC	2019 – Present
<ul style="list-style-type: none">• Metabolic engineering of thermoacidophilic Archaeon <i>Sulfolobus acidocaldarius</i>• Investigation chemolithoautotrophic growth in thermoacidophilic Order Sulfolobales by sulfur oxidation• Use of bioinformatics tools for comparative genomic evaluations• Leverage comparative growth evaluation and transcriptomics to evaluate phenotypic variations• Operation of bioreactors on 2L to 20L scales for generation of biomass and protein• Isolation of recombinant protein in <i>E. coli</i> using induced expression and FPLC purification• Maintain lab operations as Safety Officer, Hazardous Waste Manager, and Lab Purchasing Coordinator	
<i>R&D Engineering Intern</i> , Novozymes through Qualified Staffing , Franklinton, NC	Summer 2021
<ul style="list-style-type: none">• Design and implementation of experiments to address and evaluate specific client needs• Screening of enzyme candidates for third-party processing applications• Investigation of analytical method for protein distribution in process streams	
<i>Chemist Engineer I</i> , Merck Pharmaceuticals through ExecuPharm , Rahway, NJ	2017-2018
<ul style="list-style-type: none">• Member of the Reaction Engineering Lab• Investigated methods for predictive modeling of kinetics for API synthesis chemistry• Qualified in-line process analytical technology (PAT) for monitoring reaction progress specific reaction steps• Supported Pilot Plant in qualification of reaction steps and PAT monitoring	
<i>Process Engineer</i> , Avery Dennison , Painesville, OH	2015 – 2017
<ul style="list-style-type: none">• Associate in the Leadership Development Program• Engineering support for twelve web handling machines, two adhesive coaters, and one adhesive extruder• Managed \$400K capital project for installation of flammability analyzers on two adhesive coaters• Established process settings and operating procedures for roll editor, resulting in 30% improvement in editor effectiveness• Integrated automated recipe management system in Finishing• Managed/Implemented quality system databases for ISO9000 audit• Established VBA-based scheduling tool to predict and minimize changeover downtime and scrap• Led/Participated in multiple Lean Six Sigma Kaizen events for process improvement	
<i>Senior Design</i> , Bucknell University , Lewisburg, PA in association with Vertex Pharmaceutical	Spring 2015
<ul style="list-style-type: none">• Derived and validated a predictive model for mixing endpoint of powdered viscoelastic polymers mixtures• Constructed and implemented novel optical light based instrument for measurement of mixing quality	
<i>Engineering Intern</i> , Diversified CPC International , Channahon, IL	Summer 2014
<ul style="list-style-type: none">• Process Hazard Analysis of plant systems for OSHA• Analyzed and presented on material properties of plant storage tanks under various operating conditions	

- Operation of 2.5 grade 2-butene isomer fractionation

Engineering Intern, KLH Engineers, Inc., Pittsburgh, PA

Summer 2013

- Results analysis of biological nutrient reduction process for wastewater treatment
- Assessment of water treatment compliance in response to DEP violation
- Analysis of disinfection byproduct reduction in water treatment

Undergraduate Research, Bucknell University, Lewisburg, PA

Spring 2013

- Assessed mechanical properties of tung oil-based polymers using different co-monomers
- Assessed feasibility of composite materials using organic fillers in viscous co-monomer

Technical Skills

- Proficient in MATLAB, VBA, and RStudio programming environments
- Experience with Aspen HYSYS, Minitab, AutoCAD, WaterCAD
- Green Belt training in Lean Six Sigma principles
- Experience with unit operations including distillation column, spray dryer, gas-gas membrane separation, filter press, adhesive coating, web slitting, FPLC, and bioreactors ranging from 2L to 20L
- Experience with analytical equipment including SEM, NMR, GC, HPLC, LC/MS, dynamic mechanical analyzer, and FTIR

Publications

Willard, D.J. and R.M. Kelly (2021). "Evaluating the Energetics of Sulfur Oxidation in the Thermoacidophilic Order *Sulfolobales* and its Impact on Growth in *Sulfolobus acidocaldarius*." *J. Phys. Chem. B.* **125**(20): 5243-5257.

Counts, J.A., D.J. Willard, and R.M. Kelly (2021). "Life in Hot Acid: A Genome-Based Reassessment of the Archaeal Order *Sulfolobales*." *Environ. Microbiol.* **23**(7): 3568-3584.

Lewis, A.M. *et al.* (2021). "The Biology and Biotechnology of Archaeal Extreme Thermoacidophiles." *FEMS Microbiol. Rev.* **45**(4): 1-60.

Laemthong, T. *et al.* (2022). "Enzymes from Extremely Thermophilic Bacteria and Archaea: Current State and Future Prospects." In *Extremozymes and their industrial applications*.

Cooper, C. *et al.* (Submitted 2022). "Interplay between Transcriptional Regulators and VapBC Toxin-Antitoxin Loci During Thermal Stress Response in Extremely Thermoacidophilic Archaea." Under review in *Environ. Microbiol.*

Bing, R.G. *et al.* (Submitted 2022). "Fermentative Conversion of Unpretreated Plant Biomass: A Thermophilic Threshold for Indigenous Microbial Growth." Under review in *Bioresour. Technol.*

Awards and Memberships

- Member, Alpha Lambda Delta Honors Society
- Member, Tau Beta Pi Honors Society
- Robert E. Slonaker Jr. Memorial Award (2015): for outstanding achievement in the field of materials science and engineering
- Finalist for Praxair Exceptional Teaching Assistant Award (2019)
- NIH Molecular Biotechnology Traineeship (2019)

Sunyoung Woo

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Education and Training

North Carolina State University Raleigh, NC
Doctor of Philosophy in Chemical and Biomolecular Engineering August 2018 – Present

Dankook University Yongin, South Korea
Master of Science in Chemical Engineering March 2014 – August 2016
Bachelor of Science in Chemical Engineering March 2009 – February 2014

Professional Experience

North Carolina State University Raleigh, NC
Graduate Research Assistant under Prof. Jan Genzer January 2019 – Present

- Developed surface-attached polymer networks with tailorable characteristics using thermally/UV active crosslinker
- Synthesized and characterized gradient surfaces of polymer brush
- Developed methods for anchoring hydrogel to elastomer supports through chemical modification of interfaces

Dankook University Yongin, South Korea
Research Assistant under Prof. Hwankeyu Lee October 2013 – August 2016

- Performed molecular dynamics simulations of amphiphilic peptides with lipid bilayers to reveal the effect of lipid shape on pore formation and peptide orientation.
- Investigated differences between melittin peptide and its analogue MelP5 in lipid bilayers using molecular dynamics simulation.
- Simulated synthetic coiled-coil peptides for membrane fusion with lipid bilayer to calculate free energies of binding and examine differences between peptides.
- Performed molecular dynamics simulations of trimeric α -helical coiled coils grafted with poly(ethylene glycol) (PEG) and their self-assembled micelles to investigate conformation of PEGs grafted to α -helical coiled coils and measure the size of micelles.

Publications (5 first-authored, 2 co-authored)

- Ko, Y., Truong, V. K., **Woo, S. Y.**, Dickey, M. D., Hsiao, L., & Genzer, J. “Counterpropagating Gradients of Antibacterial and Antifouling Polymer Brushes”, *Biomacromolecules*, 2021, 23, 1, 424-430.
- **Woo, S. Y.**, Pandiyarajan, C. K., & Genzer, J. “Tuning the Properties of Surface-Anchored Polymer Networks by Varying the Concentration of a Thermally Activated Cross-Linker, Annealing Time, and Temperature in a One-Pot Reaction”, *ACS Applied Polymer Materials*, 2021, 3, 11, 5568-5577.
- Jang, J. G., **Woo, S. Y.**, Lee, H., Lee, E., Kim, S. H., & Hong, J. I. “Supramolecular functionalization for improving thermoelectric properties of single-walled carbon nanotubes–small organic molecule hybrids”, *ACS Applied Materials & Interfaces*, 2020, 12, 46, 51387-51396.
- **Woo, S. Y.**, Lee H., “Effect of lipid shape on toroidal pore formation and peptide orientation in lipid bilayers.” *Physical Chemistry Chemical Physics*, 2017, 19:21340-21349.
- **Woo, S. Y.**, Lee H, “Aggregation and insertion of melittin and its analogue MelP5 into lipid bilayers at different concentrations: effects on pore size, bilayer thickness and dynamics.” *Physical Chemistry Chemical Physics*, 2017, 19:7195-7203.
- **Woo, S. Y.**, Lee H, “All-atom simulations and free energy calculations of coiled-coil peptides with lipid bilayers: the binding strength, structural transition, and effect on lipid dynamics.” *Scientific Reports*, 2016, 6:22299.
- **Woo, S. Y.**, Lee H, “Molecular dynamics studies of PEGylated α -helical coiled coils and their self-assembled micelles.” *Langmuir*, 2014, 30:8848-8855.

Skills

Characterization: Ellipsometer, Fluorescence/Optical Microscope, FT-IR spectroscopy, FT-IR microscopy, Time-of-Flight Secondary Ion Mass Spectrometry, Goniometer, Profilometer

Programming: GROMACS, MATLAB, Microsoft Offices

Teaching: Teaching Assistant for Chemical Engineering capstone design (GROMACS), Thermodynamics I & II

Award and Honors

The best paper award in Dankook University	2014, 2016
Award for Excellent Graduation Records, Dankook University	2014
Merit-based Scholarship, Dankook University	2009-2013, 6 semesters

Selected Conference Presentations and Posters

- **Woo, S. Y.**, Ko, Y., Genzer, J., “Counter-propagating gradients of antibacterial & antifouling brushes”. Poster, 2022, Triangle Soft Matter Workshop, NC
- **Woo, S. Y.**, Lee, H., “MD Simulations and Free Energy Calculation of Synthetic Coiled-Coil Peptides with Lipid Bilayers”, Poster, 2016, Biophysical Society Meeting, CA
- **Woo, S. Y.**, Lee, H.,” Molecular Dynamics Studies of PEGylated α -Helical Coiled Coils and Their Self-Assembled Micelles”, Poster, 2015, Biophysical Society Meeting, MD

Z. BEGUM YAGCI

EDUCATION

NORTH CAROLINA STATE UNIVERSITY (PhD Candidate)

Department of Chemical & Biomolecular Engineering

PhD Thesis: *An In Vitro* Human Platform to Efficiently Study Angelman Syndrome Class I/II Deletion Genes

Advisor: Dr. Albert Keung

RALEIGH, NC, USA

Aug 2019 - Present

BOGAZICI UNIVERSITY (MS)

Department of Chemical Engineering

MS Thesis: *In Silico* Analysis of Neutral Sphingomyelinase 2

Advisor: Dr. Kutlu Ulgen

Co-Advisor: Dr. Elif Ozkirimli

ISTANBUL, TURKEY

Sept 2016 - Aug 2018

BOGAZICI UNIVERSITY (BS with High Honors)

Department of Chemical Engineering

Graduation Project: Investigation of the Role of Drug Transporter Qdr2p in Copper Transport

Advisor: Dr. Betul Kirdar

ISTANBUL, TURKEY

Sept 2011 - June 2016

ACADEMIC & PROFESSIONAL EXPERIENCES

Research and Teaching Assistant at NC State University, USA, Aug 2019-Present

Research Assistant in Ulgen and Ozkirimli Labs at Bogazici University, Istanbul/Turkey, Sept 2016-July 2019

Production Department Intern at TUPRAS (Turkish Petroleum Refineries Corporation), Kocaeli/Turkey, July 2015

Research & Development Laboratory Intern at BASF, Construction Chemicals Division, Kocaeli/Turkey, Aug-Sept 2014

Quality Assurance/Control Department Intern at Novartis, Istanbul/Turkey, June-July 2014

PUBLICATIONS

Journal Articles

Kazan, F., Yagci, Z. B., Bai, R., Ozkirimli, E., Hamel, E., & Ozkirimli, S. (2019). Synthesis and biological evaluation of indole-2-carbohydrazides and thiazolidinyl-indole-2-carboxamides as potent tubulin polymerization inhibitors. *Computational Biology and Chemistry*, 80, 512-523. <https://doi.org/10.1016/j.compbiolchem.2019.05.002>

Yilmazer, B., Yagci, Z. B., Bakar, E., Ozden, B., Ulgen, K., & Ozkirimli, E. (2017). Investigation of novel chaperones for Gaucher disease. *Journal of Molecular Graphics and Modelling*, 76, 364-378. <https://doi.org/10.1016/j.jmngm.2017.07.014>

Book Chapters

Yagci, Z. B., Esvap, E., Ozkara, H. A., Ulgen, K., & Ozkirimli, E. (2019). Inflammatory response and its relation to sphingolipid metabolism proteins: Chaperones as potential indirect anti-inflammatory agents. In *Advances in Protein Chemistry and Structural Biology (APCSB)*. Academic Press. <https://doi.org/10.1016/bs.apcsb.2018.09.004>

Conference Publications/Presentations

Estridge, R. C.*, Yagci, Z. B.*, Sen, D.*, Simon, J., Keung, A. J., "Identifying Cell-Type Composition Differences Between Neurotypical and UBE3A Deletion Human Cerebral Organoids with Single Cell Transcriptomics", ACS Spring 2022, 24 March 2022, San Diego, CA/USA. (Joint talk with R. Chris Estridge) *Co-first authors

Yagci, Z. B., Drobna, Z., Stuppy, S., Sen, D., Liu, H., Simon, J., Keung, A. J., "An In Vitro Human Platform to Efficiently Study Angelman Syndrome Class I/II Deletion Genes", ACS Spring 2022, 22 March 2022, San Diego, CA/USA. (Oral Presentation)

Yagci, Z. B., Drobna, Z., Stuppy, S., Sen, D., Liu, H., Simon, J., Keung, A. J., "An In Vitro Human Platform to Efficiently Study Angelman Syndrome Class I/II Deletion Genes", FAST Translational Research Symposium and Angelman Syndrome Biomarker and Outcome Measure Consortium Meeting, 2-4 December 2021, Austin, TX/USA. (Poster)

Yagci, Z. B., Drobna, Z., Stuppy, S., Sen, D., Liu, H., Simon, J., Keung, A. J., “*An In Vitro Human Platform to Efficiently Study Angelman Syndrome Class I/II Deletion Genes*”, 5th International Conference on Epigenetics and Bioengineering (EpiBio), 4-6 November 2021, Virtual. (Poster)

Estridge, R. C.*, Yagci, Z. B.*, Sen, D.*, Simon, J., Keung, A. J., “*Identifying Cell-Type Composition Differences Between Neurotypical and UBE3A Deletion Human Cerebral Organoids with Single Cell Transcriptomics*”, Modeling the Living Embryo Retreat of Quantitative and Computational Developmental Biology at NC State, 28 September 2021, Virtual. (Joint talk with R. Chris Estridge) *Co-first authors

Yagci, Z. B., Ozkirimli Olmez, E., Ulgen, K. O., “*In Silico Identification of Possible Pharmacological Chaperones for Neutral Sphingomyelinase 2*”, 19th International Conference on Systems Biology, 28 October - 1 November 2018, Lyon/France. (Poster)

Yagci, Z. B., Ozkirimli Olmez, E., Ulgen, K., “*Comparative In Silico Analysis of Bacterial and Human Neutral Sphingomyelinases*”, EMBO at BASEL LIFE, 11 - 14 September 2018, Basel/Switzerland. (Poster)

Yagci, Z. B., Ozkirimli Olmez, E., Ulgen, K. O., “*Structural and Dynamical Analysis of Bacterial and Human Neutral Sphingomyelinases*”, Glycolipid and Sphingolipid Biology Gordon Research Conference, 11 - 16 February 2018, Galveston, TX/USA. (Poster)

Esvap, E., Yagci, Z. B., Ozkirimli Olmez, E., Ulgen, K. O., “*Identification of Mutual and Specific Ligands Interacting with the Proteins in Sphingolipid and Inflammation Pathways Using a Data Mining and Network Modeling Approach*”, Glycolipid and Sphingolipid Biology Gordon Research Conference, 11 - 16 February 2018, Galveston, TX/USA. (Poster)

Yagci, Z. B., Ozkirimli Olmez, E., Ulgen, K. O., “*Structural and Dynamical Analysis of Bacterial Neutral Sphingomyelinase*”, XII Sphingolipid Club Meeting, 7 - 10 September 2017, Trabia/Italy. (Poster)

PROJECTS

An In Vitro Human Platform to Efficiently Study Angelman Syndrome Class I/II Deletion Genes

Principal Investigator: Dr. Albert Keung
Foundation for Angelman Syndrome Therapeutics, Sept 2020-Present

Structural and Dynamical Analysis of Sphingolipid Metabolic Enzymes with Special Focus on Neutral Sphingomyelinase 2

Principal Investigator: Dr. Kutlu O. Ulgen
Scientific and Technological Research Council of Turkey (TUBITAK), Grant Number: 115S208, Aug 2017-Sept 2018

Investigation of the Role of Drug Transporter Qdr2p in Copper Transport

Principal Investigator: Dr. Betul Kirdar
Scientific and Technological Research Council of Turkey (TUBITAK) 2009-A 2015/1

HONORS AND AWARDS

Praxair Teaching Fellow, Sept 2021

Linde Exceptional Teaching Assistant Award, Sept 2021

NC State College of Engineering Summer Graduate Merit Award (SGMA), Summer 2021

NC State University Provost's Doctoral Fellowship, Aug 2019 - July 2020

BS Degree in Chemical Engineering with High Honors, June 2016

COMPUTER SKILLS

MATLAB, R, C Programming, LaTeX, Linux OS, Desmond, VMD, PyMOL, ChemCAD