Schoenborn Research Symposium

Tuesday, October 3, 2023

8:15 AM - 6:00 PM

NC State McKimmon Center

Judged Competitions of Student Research

NC STATE UNIVERSITY

Chemical and Biomolecular Engineering

A Special Thanks To:

The graduate and undergraduate student presenters

CBE Department and The McKimmon Center Staff

External judges:
Dr. Javier Grajeda (Eastman) and Dr. Barclay Satterfield (Eastman)

Internal Judges:
Professors Milad Abolhasani, Sindee Simon,
Wentao Tang, and Phil Westmoreland

<u>Support and Exhibitors</u>

Linde Corporation

Environmental Protection Agency

Edward M. Schoenborn Graduate Student Fund,
established by **Russ and Susie O'Dell**, for awards

Schoenborn 2023 Research Symposium

7:45 – 8:30 AM Continental Breakfast / Welcome

8:30 – 10:00 AM Oral Presentations Session I: Biotechnology I

8:30 AM **Alison Waldman** *Comprehensive Mapping and Characterization of Histone Acetyltransferases*

8:45 AM **James Lichty** *Hormesis-Like Interactions between Amyloid β and Environmental Stressors in C. elegans, Mediated by Key Stress Response Pathways*

9:00 AM **Noor Mohammad** *CRISPR-Cas12a-Based Point-of-Care Detection Using dsDNA as Inexpensive and Nonfluorescent Reporter Molecule*

9:15 AM **Ryan Kilgore** *Peptide-Based Affinity Ligands for the Platform Purification of Next-Generation Biotherapeutics and Gene-Editing Products*

9:30 PM **R. Chris Estridge** *UBE3A Loss Broadly Impacts the Composition and Cell-Type Specific Gene Expression of Human Cerebral Organoids*

9:45 AM **Zach Hetzler** *Rapid Adeno-Associated Virus Vector Genome Quantification with Amplification-Free CRISPR-Cas12a Diagnostics*

10:30 – 11:45 PM Oral Presentations Session II: Materials

10:30 AM **Prottasha Sarker** *Enhancing Collagen Hydrogel Rheology and Injectability with Plant-derived Tannic Acid Particles: pH-dependent Interactions*

10:45 AM **Oindrila Hossain** *Rapid Vegetable Species Classification by a Low-Cost Needle-Integrated VOC Sensor Device*

11:00 AM **Mariam Sohail** *Cellulose Acetate Stabilized Pickering Emulsions for Agricultural Applications*

11:15 AM **Sneha Mukherjee** *Rational Design of Colloidal Interactions for Microbioassays and Data Storage*

11:30 AM **Pallav Jani** *Friction Reduction at Soft Interfaces under Adhesion and Load Compliance*

12:00 – 2:00 PM Lunch

12:45 PM **Keynote Address: Dr. Bruce Locke, Florida State University**

Some Highlights of My Journeys through Southeast Asia, the USA, and Europe in Life, Education, Engineering Research, and Administration

2:00 – 3:00 PM Oral Presentations Session III: Biotechnology II

2:00 PM **Ravi Appalabhotla** *Model-Guided Characterization and Manipulation of Phospholipase C-γ1 (PLCγ1) Activation*

2:15 PM **Joseph Koelbl** *Phase Field Model to Study Integrin Based Signaling and Fibroblast Haptotaxis*

2:30 PM **Ryan Bing** *Sustainable Bioproducts in an Electrified Non-Fossil Future: Plant Biomass Conversion by Fermentative Thermophiles*

2:45 PM **Daniel J Willard** *Starting the Brimstone Diet: The Enzymatic and Energetic Requirements for Engineering Sulfur Oxidation in Thermoacidophiles*

3:15 – 4:00 PM Oral Presentations Session IV: Computational, Kinetics, and Catalysis

3:15 PM **Matthew A. Dorsey** *Computational Studies of the Phase Behavior of Dipolar Colloids in the Presence of an External Field*

3:30 PM **Sherafghan Iftikhar** *Sustainable Conversion of Carbon Dioxide and Shale Gas via a Thermochemical Cyclic Redox Scheme*

3:45 PM **Michael J. Petrecca** *Enabling Li-S Batteries via Novel Multifunctional Dendritic Battery Separators*

4:00 – 6:00 PM Poster Session and Mixer

Keynote Presentation

Some Highlights of My Journeys through Southeast Asia, the USA, and Europe in Life, Education, Engineering Research, and Administration

Prof. Bruce Locke

Department Chair, Chemical and Biomedical Engineering,
FAMU-FSU College of Engineering
Distinguished Research Professor, Florida State University

In this short presentation, I would like to convey how my childhood experiences living and traveling in Southeast Asia have influenced my career as an academic and administrator, and how my education prepared me for the technical challenges in engineering. As a student, I benefited from some of the best teachers and professors one could have for a career in chemical engineering, including Professor Ruben Carbonell, my PhD advisor at NCSU, as well as my high school chemistry and calculus teachers and my MS thesis advisor. As a professor, I have worked with outstanding students and colleagues from over a dozen countries primarily spanning Asia and Europe. My students have become leaders in industry and academia. I received outstanding mentorship from colleagues in Japan, Canada, the Czech Republic, and the USA who helped me at critical times in my development as a professor. I have been awed by the excellent of my students and colleagues and glad that I could help them along their journeys. As a department chair, I have hired and helped develop our faculty from many countries and diverse backgrounds and have developed programs such as our biomedical engineering undergraduate and graduate degrees and other special programs for international students. As an associate provost at Florida State University, a large institution with broad national and international interests, I had purview over a wide range of international activities from university exchange programs to various study abroad centers as well as international visiting scholars and other activities. Throughout my professional and personal life, I have strived for a broad perspective on the world and its people, and for this I am thankful for the inspiration of my father who saw the worst of the 20th century as a child, soldier, and government official while remaining an eternal optimist.

Biography: Bruce R. Locke is a Distinguished University Research Professor at Florida State University and Chair of the Department of Chemical and Biomedical Engineering at the FAMU-FSU College of Engineering where he has been a faculty member since 1989. He earned his B.E. with double major in Chemical Engineering and Environmental and Water Resources Engineering from Vanderbilt University in 1980, M.S. degree in Chemical Engineering from the University of Houston in 1982 with Professor Neal R Amundson and his Ph.D. in Chemical Engineering from North Carolina State University under the supervision of Professor Ruben G. Carbonell in 1989. He worked on studies of ultrafine aerosol particles at the Research Triangle Institute in the Research Triangle Park between his MS and PhD studies and is a registered professional engineering in North Carolina. As a faculty member he has taught all departmental courses in transport phenomena and reaction engineering at the graduate and undergraduate levels as well as bioengineering, research methods, and advanced mathematics at the graduate level and mass and energy balances at the undergraduate level. He was awarded the Tau Beta Pi Excellence in Teaching Award. As a department chair (2004-2012 and 2019-present), he hired 15 of the current 23 permanent faculty members, led the development and accreditation of the BS degree in biomedical engineering, and helped lead and develop the department from 5 faculty members, 6 seniors and 5 graduate students in1989 to 23 faculty members, over 520 undergraduate students, and 65 graduate students presently. He served as Associate Provost at Florida State University (2012-2018) with responsibilities for international educational activities, among other duties, and he was the Interim Dean of the FAMU-FSU College of Engineering (2015-2016) where he directed a major college facilities renovation project and oversaw the ABET accreditation review.

His current research interests include plasma reaction engineering for chemical synthesis and environmental pollution control, with particular emphasis on gas-liquid plasma reactor design and development. Dr. Locke has published 144 peer reviewed journal papers and 8 book chapters with over 13,500 citations. He holds 10 US patents of which 7 are currently licensed for applications in agriculture. He has supervised 37 MS/PhD students, 21 honors undergraduate students, over 50 other undergraduate researcher projects, and 18 visiting scholars and postdocs. His students are faculty members at US and international universities and engineers and leaders in major corporations. He was a visiting professor in Japan, France, and China, and was a US Fulbright Research Scholar at the Institute of Plasma Physics, Czech Academy of Sciences. He is a Fellow of the American Institute of Chemical Engineers and co-Editor-in-Chief of the journal Plasma Chemistry and Plasma Processing published by Springer Nature.

List of Poster Presentations

Biotechnology

Cyrus Cao (G1) *Charge-induced Selective Permeability of Viral Capsids by Ionic Molecular Species*

Charles Kaleb Decker (G7) *Enabling RNA Uptake in Caenorhabditis elegans for Genetic Manipulation*

Mohamad Javad Haghighat Manesh (G6) *Recovery of Critical Metals and Rare Earth Elements Using Thermoacidophilic Archaea*

Gautami Kelkar (G5) *Investigating the Effect of Glucose Metabolism on Stress and Differentiation in Human Cerebral Organoids*

Hrishikesh Mane (G2) *Understanding the Relation Between Neuronal Activity, Reactive Oxygen Species (ROS) and Oxidative Stress Resistance Using C. Elegans*

William Smith (G3) *Development of Novel Peptide Ligands for the Purification of AcMNPV Baculovirus*

Victoria Yarmey (G4) *Investigating the Mechanisms Underlying Sensory Perception & the Neuronal Contribution to the Oxidative Stress Response*

Catalysis

Tim Mallo (G8) *Kinetic Model for the Thermal Destruction of Perfluorooctanoic Acid*

Negin Orouji (G9) *A Self-Driving Catalysis Lab for Accelerated Development of Homogeneous Catalysts*

Computational

Michael Bergman (G11) *A Computational Approach to Designing Plastic-Binding Peptides*

Sina Jamalzadegan (G10) *Machine Learning for Sensor Data Integration and Quantitative Early Detection of Plant Diseases*

Karthik Sinha (G12) *Coil-to-Helix Transitions in Polyelectrolytes*

Materials

Elaheh A. T. Moghadam (G30) *The Glass Transition in Indomethacin/Sucrose Benzoate Co-Amorphous Drug Delivery Systems*

Mesbah Ahmad (G15) *Novel Biodegradable and Stretchable Films for Soft Electronics Made of Plasticized Chitosan Biopolymer*

Muhammed Ziauddin Ahmad Ebrahim (G22) *MOF-based hybrid aerogels for enhanced functionality*

Abhirup Basu (G14) *"Moonwalking" Active Colloidal Rollers with Organized Nanoparticle Chains*

Kevser Hilal Bektas (G25) *A Novel System for High-temperature Thermal Energy Storage: Oxide-Molten Salt Composites (OMS)*

Nate Brown (G29) *Surface-Initiated ATRP Using Gelatin-Based Materials as Transfer Mediums and Reducing Agents*

Fernando Delgado-Licona (G16) *Dynamic Exploration of Quantum Dot Synthesis in a Continuous Flow Reactor*

Nidhi Diwakar (G18) *New Modes of Active Particle Propulsion Remotely Powered by AC fields*

Haeleen Hong (G19) *A New Method for Efficient Microplastic Remediation Utilizing Self-Propelling and Self-Dispersing Active Microcleaners*

Sahel Mohammadkhah (G26) *Thermal Properties of Liquid Crystals*

Nikolai Mukhin (G21) *A Material-Efficient Materials Acceleration Platform for Fast-Tracked Exploration of Colloidal Quantum Dots*

Anicah O'Brien (G24) *Effect of Surface Coatings on Biodegradability and Functional Properties of Pure and Blended Biopolymer Substrates*

Sina Sadeghi (G20) *Autonomous Nanomanufacturing of Lead-Free Metal Halide Perovskite Nanocrystals Using a Self-Driving Fluidic Lab*

Nazanin Shakoury (G23) *Impact of Nanoparticles Reinforcement on Polysulfone*

Logan Williams (G28) T*he Kinetics of Crystallization and the Rigid Amorphous Fraction of Poly(L-lactide)*

Pedro Henrique Wink Reis (G27) *Wearable Ionotronic Tactile Sensors from Sustainable Homocomposite Hydrogels*

Jinge Xu (G13) *Data-Driven Synthesis of Metal Halide Perovskite Nanocrystals with an Intelligent Multi-Robotic Platform*

Jiangfeng Xu (G17) *Phosphate Removed by Polyethylene Imine/Poly (Methyl Vinyl Ether-Alt-Maleic Anhydride) Hydrogels*

Lucille Verster (G31) Millifluidic *Flow Device for Accelerated Degradation Studies of Nonwovens*

Undergraduate Research

Daisy Aguilar Aguilar (UG8) *CHTXS: An Automated Detector Program for Data Analysis of Chemotaxis Assays*

Hannah F. Dickerson (UG3) *Process Intensification Through Data-Rich Approach: Dynamic Exploration of Continuous Flow Quantum Dot Parameter Space*

Jenna Kolbe (UG1) *Scalable Expression of LbCas12a Proteins in E. Coli*

James Z. Kurdi (UG5) *Tunable Gradient Development Enables Exploration of Context-Dependent Cell Migration*

Hrishikesh Ram (UG9) *Thermochemistry of Species in Gas-Phase Thermal Oxidation of C2 to C8 Perfluorinated Carboxylic Acids*

Elijah Rushing (UG7) *Risk Integration and Comparison Safety Study Between Generation II Light Water Reactors and Generation IV Non-Light Water Reactors*

Amelia L. Shea (UG6) *Understanding the Glass Transition Temperature of Felodipine/Cholic Acid Co-Amorphous Systems*

Christine Stark (UG4) *High-Throughput Single-Cell Sequencing of B. Fragilis Populations in the Mouse Gut*

Katie Traynelis (UG2) *High Throughput Mapping of Epigenetic Enzyme Activity*

Abstracts for Oral Presentations

Comprehensive mapping and characterization of histone acetyltransferases

Alison Waldman [1], Albert Keung [1], Balaji Rao [1, 2]

1. Dept. of Chemical and Biomolecular Engineering, North Carolina State University; 2. Golden LEAF Biomanufacturing Training and Education Center (BTEC), North Carolina State University

Background: Eukaryotic DNA is organized into chromatin, which consists of DNA, histones, and other associated proteins. Human histone proteins are decorated with a combinatorially and numerically diverse set of biochemical modifications. Various genomic functional states are modulated or even defined by specific epigenomic landscapes, making them of utmost importance for our full understanding of cell biology. Distinct histone modification patterns are dynamically regulated by a cohort of epigenomic enzymes that write, read, and erase these biochemical marks. The work presented here seeks to expand the engineering tool kit available to chromatin biologists to study these epigenomic enzymes.

Results: Traditional methods to study histone modification patterns and the epigenomic enzymes that regulate them have transformed the field of chromatin biology. However, each method has its limitations and can be laborious, time consuming, and cumbersome at times. Using yeast surface display we established a versatile and scalable platform, REMY (Rapid interrogation of Epigenomic Modifications using Yeast) [1]. REMY enables efficient characterization of the enzymes that create histone modifications without the need for recombinant protein production. We used REMY to map the residue specificities of several human histone acetyltransferase proteins on multiple human histones. We have also expanded the utility of our platform to uncover the relationship between substrate protein sequence and the catalytic activity of epigenomic enzymes. We aim to use the information gathered from our experiments to accelerate our protein engineering efforts to create a designer acetyltransferase.

Conclusions: REMY is a versatile and robust platform that connects the powerful protein engineering and screening abilities of yeast surface display with chromatin biology. Since only standard molecular biology, yeast culture, and flow cytometry analyses are required, our platform provides a potentially democratizing, cost-effective, and time efficient platform for studying chromatin biology and epigenomic enzymes. Our results show that using REMY to study histone modifications can not only advance our understanding of the natural proteins that regulate chromatin biology but also enable us to engineer advanced epigenomic enzymes for use in transcriptional control and cellular engineering.

References:
1. Waldman, Alison C., Rao, Balaji M., and Alber J. Keung (2021). Mapping the Residue Specificities of Epigenome Enzymes by Yeast Surface Display. *Cell Chemical Biol.*, 12: 1772-1779.

Hormesis-Like Interactions Between Amyloid β and Environmental Stressors in C. elegans, Mediated by Key Stress Response Pathways

James Lichty [1], Adriana San Miguel [1]
1. Dept. of Chemical and Biomolecular Engineering, North Carolina State University

Background: Alzheimer's Disease (AD) is a neurodegenerative disorder characterized by a progressive loss of mental and physical capabilities in those afflicted with it [1]. AD is identified by many abnormalities in the brain, such as widespread oxidative stress, immunity activation, neurodegeneration, inflammation, and protein aggregation [2]. Amyloid β (Aβ) has been implicated in the disease through the association of Aβ's accumulation and aggregation with various AD traits [2]. To study of the role of this peptide in AD, several models using the organism *C. elegans* have been engineered to express Aβ pan-neuronally [3,4]. Previous work with these models has shown Aβ's ability to aggregate and induce oxidative stress, neurodegeneration, and reduced lifespan in *C. elegans*, but there are several other ways in which Aβ may influence worm health [3,4]. Environmental stressors, including heat stress, oxidative stress, starvation, and hypoxia, are known to significantly impact worm health, but their interactions with Aβ have been largely unexplored. This work focuses on elucidating how Aβ impacts worm health and survival in response to severe environmental stressors.

Results: We initially hypothesized that exposure to an external stressor while under the effects of Aβ would act synergistically to the detriment of the worm's health. By exposing Aβ-expressing *C. elegans* to an oxidative stressor, paraquat, we show Aβ lowers oxidative stress resistance. Contrary to expectations though, Aβ expression increases resistance to several other stressors, indicating a possibly hormesis-like effect. Additionally, we show, with a temperature inducible Aβ, a correlation between Aβ levels and heat stress resistance. By expressing Aβ in different tissues, we show that this is a neuron-specific effect. Using gene-expression analysis techniques, we identified several stress response pathways that are affected by Aβ expression. Using targeted gene suppression, we validated those results and confirmed several gene's role in this effect.

Conclusions: Through this work we have shown that Aβ induces several stress response pathways when expressed pan-neuronally in *C. elegans*. This produces a hormesis-like effect in the worms which selectively increases resistance to certain stressors, while decreasing resistance to other. Our results improve the understanding of how Aβ influences *C. elegans* and allow for better experimental design and data interpretation in future work.

References:

1. *What is Alzheimer's Disease? | CDC*. (n.d.). Retrieved November 23, 2020, from https://www.cdc.gov/aging/aginginfo/alzheimers.htm

2. Pimplikar, S. W. (2009). Reassessing the amyloid cascade hypothesis of Alzheimer's disease. *International Journal of Biochemistry and Cell Biology* (Vol. 41, Issue 6, pp. 1261–1268). NIH Public Access.

3. Link, C. D. (1995). Expression of human β-amyloid peptide in transgenic Caenorhabditis elegans. *Proceedings of the National Academy of Sciences of the United States of America*, *92*(20), 9368–9372.

4. Gallrein, C., et. al. (2021) Novel amyloid-beta pathology *C. elegans* model reveals distinct neurons as seeds of pathogenicity. *Progress in Neurobiology* (198).

CRISPR-Cas12a-based point-of-care detection using dsDNA as inexpensive and nonfluorescent reporter molecule

Noor Mohammad [1], Shrinivas Katkam [1], Logan Talton [1], Zach Hetzler [1], Megha Gongireddy [1], Selen Dalgan [1], Alireza Velayati [1], Shengwei Zhang [1], and Qingshan Wei [1]*

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

Background: CRISPR-diagnostics, mainly based on the trans-cleavage of single-stranded (ss) DNA reporter [1], often rely on colorimetric, fluorescent, or electrochemical signaling mechanism, which involves expensive reporters and/or sophisticated equipment [2]. To overcome these limitations in point-of-care (POC) applications, we demonstrated inexpensive, nonoptical, and sensitive CRISPR-Cas12a-based sensing platforms to detect ssDNA targets using a series of double-stranded (ds) reporter molecules [3][4].

Results: We discovered the unique trans-cleavage activity of Cas12a towards dsDNA substrates, and therefore developed a set of novel nonoptical reporters, including ds λ DNA, 3' toe-activated hybrid DNA reporters, and circular plasmid DNA reporters. Firstly, we demonstrated a simple yet sensitive CRISPR-Cas12a-based sensing platform to detect ssDNA by sizing ds λ DNA as novel reporter molecules. We hypothesized that the massive trans-nuclease activity of Cas12a toward λ DNA was due to the presence of ss looped structures along the λ DNA sequence. This DNA sizing-based signaling technique helped achieve sub-picomolar (< pM) detection sensitivity, ~100 times more sensitive than the fluorescent counterpart. Secondly, we discovered that Cas12a trans-cleaved 3' overhang dsDNA substrates at least 3 times faster than 5' overhang substrates, which unfolded unidirectional trans-cleavage behavior of Cas12a. Utilizing this new finding, we designed a hybrid DNA reporter as nonoptical substrate, which sensitively detected ssDNA targets at sub picomolar level. Finally, we developed a ratiometric CRISPR assay based on CRISPR-Cas12a-induced DNA supercoil relaxation of nonspecific circular dsDNA plasmids. This technique was rapid, sensitive, and accurate by including a self-band size calibration mechanism. Using this 3rd strategy, we demonstrated a battery-powered minigel electrophoresis device which can bring DNA size analysis to the field for true POC diagnostics.

Conclusions: Our results highlighted that certain features in dsDNA, such as ss loops or 3' toe, could facilitate the initiation of trans-cleavage, making dsDNA a new class of reporters for the CRISPR-Cas12a system. Furthermore, we unveiled the unidirectional trans-cleaving behavior of Cas12a. Of the three sensing strategies employing λ DNA, hybrid reporters, and circular DNA, the circular DNA supercoil relaxation approach demonstrated the best combination of detection sensitivity and speed. These discoveries not only enriched the current CRISPR-Dx design and also provided new insights into the CRISPR trans-cleavage biology.

References:

1. Chen, J. S., Ma, E., Harrington, L. B., Da Costa, M., et al., *Science*, 2018, 360, 436–439.
2. Mohammad, N., Katkam, S. S. and Wei, Q., *CRISPR J.*, 2022, 5, 500–516.
3. Mohammad, N., Katkam, S. S. and Wei, Q., *Angew. Chem. Int. Ed*., 2022, 61, e202213920.
4. Mohammad, N., Talton, L., Hetzler, Z., Gongireddy, M., and Wei, Q., *Nucleic Acids Res.*, 2023, gkad715.

Peptide-based affinity ligands for the platform purification of next-generation biotherapeutics and gene-editing products

Ryan Kilgore [1], Wenning Chu [1], Brandyn Moore [1], Yuxuan Wu [1], Sobhana Sripada [1], Eduardo Barbieri [1], Shriarjun Shastry [1][2], Shiqi Hu [3], Ke Cheng[3][7], Dipendra Bhandari [4], David Fischler [4], Michael Crapanzano [4], Weihua Tian [5], Steffen Goletz [5], Heidi Petersen [6], Mohammad Mohammadifar [6], Michael A. Daniele [7][8][9], Ruben G. Carbonell [1][2], Stefano Menegatti [1][2][4][9],

1. Department of Chemical and Biomolecular Engineering, North Carolina State University; 2. Biomanufacturing Training and Education Center, North Carolina State University; 3. Department of Molecular Biomedical Sciences at the College of Veterinary Medicine, North Carolina State University; 4. LigaTrap Technologies; 5. Department of Biotechnology and Biomedicine, Denmark Technical University; 6. National Food Institute at Denmark Technical University; 7. Joint Department of Biomedical Engineering, North Carolina State University and University of North Carolina at Chapel Hill; 8. Department of Electrical and Computer Engineering, North Carolina State University; 9 North Carolina Viral Vector Initiative in Research and Learning (NC-VVIRAL)

Background: The landscape of biotherapeutics is evolving rapidly, driven by innovations such as gene-delivery vectors, engineered antibody fragments, and gene-editing nucleases. While these developments signal a transformative era for healthcare, they face immense roadblocks in the form of immature purification processes. In response, our group developed a technology to rapidly discover peptide affinity ligands that are fine-tuned for target selectivity and tailored binding strengths. We then developed purification strategies for targets of increasing complexity.

Results: First, we developed peptides for the universal purification of Fab antibody fragments. These peptides demonstrated binding to both Fab kappa and lambda, while achieving high yields (~95%) and purities (93-fold reduction of host cell proteins (HCP)). These results were complemented by a robust dynamic binding capacity ($DBC_{10\%}$ up to 16 mg/mL). Second, we identified ligands that selectively bound and purified CRISPR-Cas nucleases (Cas9 and Cas12a) from *E. coli* HCPs. Finally, we present ligands capable of universally purifying exosomes from a variety of sources (14 tested) whether they were spiked into HEK293 fluid or naturally present within it. We achieved yields up to 80% with a 51-fold reduction of HCPs, utilizing mild elution conditions with moderate conductivity and physiological-to-basic pH.

Conclusions: Our research shows the potential and benefits of peptide affinity ligands in purifying next-generation, high value biotherapeutics, spanning from straightforward Fab fragments to extraordinarily diverse and unstable exosomes.

UBE3A loss broadly impacts the composition and cell-type specific gene expression of human cerebral organoids

R. Chris Estridge* [1], Z. Begum Yagci* [1], Dilara Sen* [1], Jeremy Simon# [2,3], Albert J. Keung# [1]

1. Dept. of Chemical and Biomolecular Engineering, North Carolina State University; 2. Dept. of Genetics, University of North Carolina Chapel Hill; 3. Dana-Farber Cancer Institute

*Co-first author

#Co-corresponding author

Background: *UBE3A* is an imprinted gene located on chromosome 15 that encodes the E3 ubiquitin ligase enzyme, E6AP1. While most tissues retain two functioning copies of *UBE3A*, it is expressed only from the maternal allele in neurons due to epigenetic silencing of paternal *UBE3A* [1]. Absence of maternal *UBE3A* is the common lesion driving Angelman Syndrome (AS), a neurodevelopmental disorder characterized by intellectual disability, speech impairment, ataxia, and seizures [2]. Furthermore, its overexpression has been linked to another neurodevelopmental disorder, Autism Spectrum Disorder [3]. Being implicated in the etiology of these disorders and its cell-type specific imprinting in the brain indicate that *UBE3A* dosage is critical for neurodevelopment [4]. Research on the effects of *UBE3A* has focused largely on its role in neurons due to its imprinted status in that cell type. Yet, evidence suggests there may be broader impacts of *UBE3A* dysregulation. Human cerebral organoids (hCOs) could be a useful model to investigate these understudied aspects of *UBE3A* biology. Our lab has previously shown hCOs can recapitulate *UBE3A* spatiotemporal localization and paternal silencing [5].

Results: Here we exploit hCOs to reveal the effects of *UBE3A* loss on transcriptomic and cell-type compositional effects, with potential implications for understudied impacts of *UBE3A* on neurodevelopment, non-neuronal cells, and cerebrospinal fluid biology. In this work, we performed single cell RNA-sequencing (scRNA-seq) on hCOs to study the effects of *UBE3A* disruption on cell-type and transcriptome compositions. In the absence of *UBE3A*, stem cells prematurely exited multipotency towards neuron and choroid plexus fates.

Conclusions: Our findings suggest *UBE3A* absence broadly significantly affects hCO development resulting in disrupted neuronal maturation. This work reveals novel impacts of *UBE3A* on human neurodevelopment and elucidates potential new therapeutic targets.

References:

1. Rougeulle C, Glatt H, Lalande M. The Angelman syndrome candidate gene, UBE3AIE6-AP, is imprinted in brain. *Nat Genet*. 1997;17(1):14-15. doi:10.1038/ng0997-14

2. Jiang Y, Armstrong D, Albrecht U, et al. Mutation of the Angelman Ubiquitin Ligase in Mice Causes Increased Cytoplasmic p53 and Deficits of Contextual Learning and Long-Term Potentiation. *Neuron*. 1998;21(4):799-811. doi:10.1016/S0896-6273(00)80596-6

3. Vatsa N, Jana NR. UBE3A and Its Link With Autism. *Front Mol Neurosci*. 2018;11:448. https://www.frontiersin.org/article/10.3389/fnmol.2018.00448

4. Silva-Santos S, van Woerden GM, Bruinsma CF, et al. Ube3a reinstatement identifies distinct developmental windows in a murine Angelman syndrome model. *J Clin Invest*. 2015;125(5):2069-2076. doi:10.1172/JCI80554

5. Sen D, Voulgaropoulos A, Drobna Z, Keung AJ. Human Cerebral Organoids Reveal Early Spatiotemporal Dynamics and Pharmacological Responses of UBE3A. *Stem Cell Reports*. 2020;15(4):845-854. doi:10.1016/j.stemcr.2020.08.006

Rapid Adeno-Associated Virus Vector Genome Quantification with Amplification-Free CRISPR-Cas12a Diagnostics

Zach Hetzler [1], Stella Marinakos [2], Noah Lott [3], Noor Mohammad [1], Agnieszka Lass-Napiorkowska [4], Jenna Kolbe [1], Lauren Turrentine [1], Delaney Fields [1], Laurie Overton [3], Angus Hucknall [2], Oliver Rammo [5], Helena Marie [5], Henry George [4], and Qingshan Wei [1]

1. Dept. of Chemical and Biomolecular Engineering, North Carolina State University; 2. Biostealth, Durham, NC, 27705; 3. Biomanufacturing, Training, and Education Center (BTEC), North Carolina State University, Raleigh, NC, 27606; 4. Millipore-Sigma, St. Louis, MO, 63103; 5. Merck KGaA, Darmstadt, DE

Background: Gene therapy has undergone rapid expansion of clinical application and interest due to the promising potential for curative therapies. Adeno-associated virus (AAV) vectors are one of the most widely used gene therapy delivery platforms due to their nonpathogenic property, capsid programmability, and long-term transgene expression [1]. AAV production, however, lacks innovative process analytical technology (PAT) needed for efficient process monitoring. A pressing analytical challenge is the determination the percent full AAV produced, a type of characterization required by the FDA [2].

Results: Here, we report an at-line CRISPR-Cas12a mediated vector genome quantification assay for vector analysis, delivering accurate determination of the vector genome concentration within 30 minutes. We constructed the CRISPR-Cas12a assay to specifically target the conserved inverted terminal repeats (ITRs) of the AAV genome as a potential platform AAV diagnostic approach. The CRISPR assay accurately quantified the genome titer of 2 different genomic constructs. The limits of detection for each AAV were optimized below 5e8 vg/mL with >1 log working range within 30 minutes of assay time. We also demonstrated the flexibility of AAV quantification with the CRISPR assay on-chip with pre-deposited reagents.

Conclusions: This new PAT drives down the time-to-result for gene therapy PAT while simplifying the vector genome titration workflow with a highly flexible assay format that can deliver higher throughput results than current analytical technologies.

References:

1. Wang, D. Tai, P.W.L., and Gao, G. (2019). Adeno-associated virus vector as a platform for gene therapy delivery. *Nat. Rev. Drug Discov*., **31**: 315-332.
2. Srivastava, A., Mallela, K.M.G., Deorkar, N., and Brophy, G., Manufacturing Challenges and Rational Formulation Development for AAV Viral Vectors., *J. Pharm. Sci*., **110**: 2609-2694.

Enhancing Collagen Hydrogel Rheology and Injectability with Plant-derived Tannic Acid Particles: pH-dependent Interactions

Prottasha Sarker [1], Orlando J. Rojas [2], Saad A. Khan [1]

1. Department of Chemical and Biomolecular Engineering, North Carolina State University;
2. Department of Chemical & Biological Engineering, The University of British Columbia

Background: The use of renewable materials for tissue engineering and regeneration has gained significant interest in recent years. Collagen-based systems, in particular, offer great potential as injectable hydrogels. However, collagen on its own has poor mechanical strength. In this study, plant-derived tannic acid (TA) was added to collagen in particulate form to enhance its mechanical properties and provide therapeutic functionalities.

Results: The rheology of the resulting hydrogels was monitored as a function of TA particle concentration, and it was found that the incorporation of TA particles generated a larger increase in elastic modulus compared to TA solution at similar concentrations. The hydrogels with TA particles also showed high cell viability and cellular activity, making them a promising candidate for tissue regeneration technology. Another aspect of this study is the exploration of the pH-dependent interaction behavior between collagen and TA particles. The results showed that TA particles at physiological pH provided stronger mechanical reinforcement to collagen at pH 4, due to their engagement in forming a higher extent of electrostatic interaction and hydrogen bonding compared to collagen at pH 7. The isothermal titration calorimetry (ITC) results validated this hypothesis, indicating that the interaction between collagen and TA particles is purely enthalpy-driven through electrostatic interactions and hydrogen bonding.

Conclusions: Overall, the development of this biobased hybrid hydrogel system for injectables in tissue regeneration technology can serve as a simple beneficial alternative to difficult implantation scenario. Additionally, the fundamental information critical to understanding the interaction between collagen and TA particles under different conditions can be utilized to optimize the system.

Rapid Vegetable Species Classification by a Low-Cost Needle-Integrated VOC Sensor Device

Oindrila Hossain [1,3], Yan Wang [1], Mingzhuo Li [1], Sina Jamalzadegan [1], Noor Mohammad [1,3], Aditi Dey Poonam [1], Qingshan Wei [1,2]

1. Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, NC 27695, USA; 2. Emerging Plant Disease and Global Food Security Cluster, North Carolina State University, Raleigh, NC 27695, USA; 3. Department of Chemical Engineering, Bangladesh University of Engineering and Technology, Dhaka-1000, Bangladesh

Background: Volatile organic compounds (VOCs) are a diverse group of organic chemicals that are naturally present in various fruits and vegetables. In the case of vegetables, these VOCs play a crucial role in determining their overall quality attributes, such as firmness, sweetness (soluble sugars), flavonols (a class of plant pigments with potential health benefits), and translucency. [1] While the importance of VOCs in assessing vegetable quality is appreciated, the conventional methods used for VOC detection, such as Gas Chromatography-Mass Spectrometry (GC-MS) and Proton Transfer Reaction Mass Spectrometry (PTR-MS), have some limitations. [2] These techniques require sophisticated and expensive equipment, cumbersome sample preparation, and are often time-consuming. Moreover, VOCs are often short-lived, making their detection challenging using these traditional methods. [3]

Results: We have developed a rapid and cost-effective sensor solution for quantifying vegetable VOCs at point-of-need. The system consists of a paper-based colorimetric VOC sensor array and a needle device that induces vegetable VOC release with minimal invasion of the skin of the vegetable. We have screened and optimized the colorimetric sensing elements for detecting and classifying all major sulfur-based VOCs, including sulfoxides, sulfides, mercaptans, and thiophenes, which are commonly found in vegetables. The integrated sensor platform proficiently discriminated between four vegetable subtypes originating from two major categories within 2 min of testing time.

Conclusions: This rapid and minimally invasive sensing technology holds great promise as an alternative tool for conducting field-based vegetable quality monitoring. The novel dual-functional VOC sensing platform stands out for its remarkable cost-effectiveness, with each test costing approximately $2.

References:

1. Kumar, A., M. Castro, and J.-F., Feller *Review on Sensor Array-Based Analytical Technologies for Quality Control of Food and Beverages*. Sensors, 2023. **23** (8), 4017.
2. Li, Z., et al., *Non-invasive plant disease diagnostics enabled by smartphone-based fingerprinting of leaf volatiles.* Nature Plants, 2019. **5**(8): p. 856-866.
3. Järvenpää, E.P., et al., *Determination of fresh onion (Allium cepa L.) volatiles by solid-phase microextraction combined with gas chromatography-mass spectrometry.* Zeitschrift für Lebensmitteluntersuchung und -Forschung A, 1998. **207**(1): p. 39-43.

Cellulose acetate stabilized Pickering emulsions for agricultural applications

Mariam Sohail [1], Tahira Pirzada [1], Richard Guenther [2], Eduardo Barbieri [1], Tim Sit [2], Stefano Menegatti [1], Nathan Crook [1], Charles Opperman [2], Saad A. Khan [1]
1. Dept. of Chemical and Biomolecular Engineering, North Carolina State University; 2. Dept. of Entomology and Plant Pathology, North Carolina State University

Background: Pickering emulsions offer a powerful platform to entrap functional moieties such as active ingredients (AI) for various applications. For instance, modern agriculture relies on the use of agricultural AIs, which are generally used in the form of emulsifiable concentrates containing large quantities of organic solvents and surfactants.[1] We propose an environmentally friendly alternative to emulsifiable concentrates entailing the use of cellulose acetate (CA) nanoparticles (NP) as Pickering emulsifiers to produce surfactant-free emulsions. CA is a widely used cellulose ester due to its ease of processing, biodegradability, and biocompatibility.[2]

Results: The NPs are produced from an easily scalable nanoprecipitation process and are used to stabilize a model oil/water system. The emulsions are shelf stable at NP concentrations as low as 0.5 wt.% CA. We probe the effect of CA concentration and the oil/water ratio on the emulsion rheology and stability. The emulsions display gel-like characteristics, with both storage and loss modulus being independent of frequency. Yield stress measurements demonstrate a distinct variation in the microstructure yielding behaviour with change in the NP concentration. We attempt to explain these trends based on the emulsion droplet size and distribution along with the morphology of the CA NP, correlating the rheology data with microscopic evidence. Furthermore, the emulsions are viable with two model agricultural cargo, including a hydrophobic nematicide, abamectin and a plant growth promoting microbe, *Pseudomonas simiae*. In-vitro release assays show sustained abamectin release demonstrating achievement of controlled active release. While loading of *Pseudomonas simiae* enables enhanced microbe viability with viability assays showing significantly higher microbe survivability compared to controls after storage at room temperature for ten weeks.

Conclusions: Compatibility of the emulsions with both agrochemicals and microbes holds the promise for a versatile loading platform for diverse active types for a wide range of applications. Thus, in addition to explaining the fundamental rheology of the CA emulsions, we demonstrate proof of concept of their potential as a loading platform for various cargos.

References:
1. J. Feng, et al. (2018), Nanoemulsions Formulation, Applications, and Characterization, Academic Press.
2. T. Pirzada and M. Sohail (2022), Adv. Funct. Mater. 32, 2270107.

Rational Design of Colloidal Interactions for Microbioassays and Data Storage

Sneha Mukherjee [1], Tamoghna Saha [1], Kevin N. Lin [1], Albert J. Keung [1], Michael D. Dickey [1], and Orlin D. Velev [1]

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

Background: Colloidal interactions play a pivotal role in various biological and bio-derived processes. Understanding these interactions is crucial for a broad spectrum of applications, from healthcare and pharmacology to food science and biotechnology. In the first part of our work we focus on developing wearable sensors for healthcare. 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. 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. 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). For the second part of our work, we focus on DNA nanobiotechnology. Exploring ways to harness the power of DNA as a basis for future technologies is of peak interest. The remarkable molecular interactions of DNA have facilitated the development of diverse DNA nanostructures. In our study, we have synthesized stable, well-defined DNA nanoparticles by controlling the relatively high ionic strength. We used dynamic light scattering (DLS) to investigate changes in size and charge of these salt-actuated nanoparticles based on the DNA structure (i.e., minor, and major groove, base stacking, and charged phosphate backbone) and its flexibility and adhesivity.

Results: Our LFA platform can function with very low sweat volumes (~2-3 μL) and can detect K^+ levels from human skin under moderate intensity exercise and rest. The patch could also osmotically sample sweat lactate directly from the surface of skin. 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. In the subsequent applications of these principles, we observe dynamic DNA nanoaggregation driven by ionic self-association. When exposing DNA suspensions to increasing salt environments, we observe the onset of aggregation. This eventually leads to the formation of stable, reproducible, and well-defined aggregates at high salt concentrations. This study explains the fundamentals behind the formation of these DNA nanoparticles and focuses on how size, hybridization and sequences can affect the binding. Data files could be successfully stored and retrieved from these nanoaggregates.

Conclusions: Understanding and colloidal design of the biomolecular transport and interactions in microfluidic devices enable us to develop novel non-invasive wearable patches that can enhance affordable advanced healthcare, by eliminating the need to visit medical centers for biomarker-based diagnostics. Similarly, understanding and control of the fundamentals of colloidal and surface interactions allow us to explore the capabilities of DNA based nanostructures towards future applications such as high-density and high-capacity information storage, drug-delivery and self-healing materials.

Friction reduction at soft interfaces under adhesion and load compliance

Pallav Jani [1], Saad Khan [1], Lilian Hsiao [1]
1. Dept. of Chemical and Biomolecular Engineering, North Carolina State University

Background: Friction reduction in the absence of liquid lubricants is of critical importance in emerging applications such as haptic-guided soft robotics, flexible electronics and biomedical devices. Organic slip additives are commonly used to impart polymers a slippery surface [1], but their friction reduction mechanism on soft substrates remains unclear. Additionally, there is a lack of systematic friction control strategies due to friction's multi-scale nature [2].

Results: We develop scaling relations for the friction reduction of erucamide, a widely used slip additive, with respect to the interfacial contact pressure (P) across multiple polymeric contacts spanning three orders of elastic moduli from soft textile-skin to hard polymer-metal interfaces. The frictional response of erucamide-coated interfaces was recorded using a stress-controlled triborheometer. Utilizing Bowden and Tabor's adhesive theory of friction, we identify two distinct friction dissipation regimes of multilamellar crystal-like erucamide films– (I) at low P values, an adhesion regime where the interfacial stress is pressure-independent and dictated by van der Waals forces for soft and compliant interfaces, and (II) at high P values, a load regime where the interfacial stress scales with P for stiff interfaces. This transition could be linked to pressure-induced changes in erucamide slip plane dynamics. In the adhesion regime, attractive interactions localize the slip plane between the interfacial layers, and the structure of the slip additive and the substrate compliance play a critical role in dictating the friction reduction with the more ordered slip additive (erucamide) outperforming the disordered additive (behenamide). The transition to the load regime allows breakdown of adhesive interactions which induces interlayer slippage and multiple slip planes that maximize the friction reduction of the slip additive. No further change in friction reduction is observed post transition irrespective of the slip additive structure or substrate compliance with both erucamide and behenamide demonstrating similar friction reduction.

Conclusions: The friction reduction mechanism and scaling framework of slip additives in the adhesion and load regimes developed in this work shed light on the intricate interplay of contact pressure, compliance, and additive molecular structure in determining frictional behavior, offering insights into optimizing or designing friction modifiers for various low friction-soft polymeric systems.

References:

1. Spikes, H. (2015). Friction modifier additives. *Tribology Letters*, 60, 1-26.
2. Zhang, J., & Meng, Y. (2015). Boundary lubrication by adsorption film. *Friction*, 3, 115-147.

Model-Guided Characterization and Manipulation of Phospholipase C-γ1 (PLCγ1) Activation

Ravikanth Appalabhotla [1], Priscila F. Siesser [2], Mark A. Hazelbaker [2], Mitchell T. Butler [2], James E. Bear [2], and Jason M. Haugh [1]

1. Dept. of Chemical and Biomolecular Engineering, North Carolina State University; 2. Dept. of Cell Biology and Physiology, Lineberger Comprehensive Cancer Center, University of North Carolina School of Medicine

Background: Phospholipase C-γ1 (PLCγ1) 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 PLCγ, 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 distribution. To evaluate if PLCγ1 mutants can be distinguished by their membrane dissociation kinetics in live cells, we developed an optogenetic tool, OptoPLC, that enables spatiotemporal control of PLCγ1 recruitment to the plasma membrane.

Conclusions: We identify a methodology to derive expected membrane association/dissociation statistics based on a structure-based kinetic model of PLCγ activation. Pairing these expected statistics with *in vitro* single-molecule activation experiments will offer mechanistic insight into how cancer-associated mutations enhance PLCγ activity. We also developed an optogenetic strategy to study the kinetics of PLCγ1 membrane dissociation in living cells. This framework for linking structure-based kinetic models to experiments can be adapted to investigate the activation kinetics of other autoinhibited enzymes.

References:

1. Nosbisch JL, Bear JE, Haugh JM. A kinetic model of phospholipase C-γ1 linking structure-based insights to dynamics of enzyme autoinhibition and activation. *J Biol Chem*. 2022 May;298(5):101886.
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

Phase Field Model to Study Integrin Based Signaling and Fibroblast Haptotaxis

Joseph Koelbl [1], Jason Haugh [1]

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

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 was used to implement stochastic adhesion networks with prescribed biases to exponential haptotactic gradients in Python. 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%. Additionally, denuding of the surface gradient by the cells can enhance the response of directed motility and persistence of the cell motion.

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. Additionally, this model can be used to inform experimental results and provides a framework for more complicated signaling architectures.

References:

1. King SJ, Asokan SB, Haynes EM, et al. Lamellipodia are crucial for haptotactic sensing and response. *J Cell Sci*. 2016;129(12):2329-2342. doi:10.1242/jcs.184507

Sustainable Bioproducts in an Electrified Non-Fossil Future: Plant Biomass Conversion by Fermentative Thermophiles

Ryan G. Bing [1], James R. Crosby [1], Tunyaboon Laemthong [1], Daniel J. Willard [1], Mohamad J. H. Manesh [1], Michael W.W. Adams [2], Robert M. Kelly [1]

1. Dept. of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh; 2. Dept. of Biochemistry and Molecular Biology, University of Georgia, Athens

Background: The world is moving to reduce its dependence on fossil energy by shifting to alternative electric sources. While many fossil-dependent processes can be electrified, some petroleum-derived chemicals cannot (i.e. plastics, jet fuel). Renewable, sustainable alternatives are needed for these. Biological conversion of lignocellulosic plant biomass is seen as a possible route to produce these chemicals, however, until recently, been unable to compete with fossil prices. A handful of thermophilic bacteria excel at degradation of the complex polysaccharides in lignocellulosic plant biomass. These include moderate (<70°C) and extreme (>70°C) thermophiles. Work is ongoing to better understand how these bacteria break down polysaccharides and engineer them to produce desirable products at industrial relevant levels [1].

Results: Extreme thermophily can offer advantages for plant biomass fermentation. Several aspects of this were investigated, including capacity to degrade plant biomasses [2], evaluation of contamination resistance [2], and novel production separation techniques [3]; both the extreme thermophile, *Anaerocellum bescii*, and the moderate thermophile, *Acetivibrio thermocellus*, were evaluated. While the bacteria have similar lignocellulose degradation abilities, only temperatures ≥75°C are able to resist contamination and allow separation of volatile products (acetone, ethanol) directly from fermentation headspace (bioreactive distillation) [2, 3]. An in-depth investigation into the diversity and ecology of the extremely thermophilic, (hemi)cellulolytic Caldicellulosiruptorales, established these bacteria as the sole members of their order, corresponding to their unique physiology [4]. Beyond plant biomass deconstruction, metabolic engineering efforts in *A. bescii* are underway to improve production of volatile chemicals. Significant improvements in ethanol selectivity have been achieved, but induced unexpected aggregation phenotypes. Further work to understand this and improve titers are underway.

Conclusions: Industrial feasibility and advantages of extremely thermophilic plant biomass conversion were demonstrated. Evaluation of the Caldicellulosiruptorales (phylogeny, ecology, phenotypes) provided novel insights into extremely thermophilic plant biomass deconstruction. Together these define specific metabolic engineering targets and aid in the building of more industrially relevant strains of *A. bescii* for production of volatile chemicals from plant biomass.

References:

1. R.G. Bing, et al., 2021. Thermophilic microbial deconstruction and conversion of natural and transgenic lignocellulose. *Environ. Microbiol. Rep.* 13:272-293.
2. R.G. Bing, et al., 2023. Fermentative conversion of unpretreated plant biomass: A thermophilic threshold for indigenous microbial growth. *Bioresource Technol.* 367:128275
3. R.G. Bing, et al., 2022. Plant Biomass fermentation by the extreme thermophile *Caldicellulosiruptor bescii* for co-production of green hydrogen and acetone: Technoeconomic analysis. *Bioresource Technol*. 348:126780
4. R.G. Bing, et al., 2023. Whither the genus *Caldicellulosiruptor* and the order *Thermoanaerobacterales*: phylogeny, taxonomy, ecology, and phenotype. *Front. Microbiol.* 14

Starting the Brimstone Diet: The Enzymatic and Energetic Requirements for Engineering Sulfur Oxidation in Thermoacidophiles

Daniel J. Willard, Mohamad J.H. Manesh, Ryan G. Bing, April M. Lewis, and Robert M. Kelly
Dept. of Chemical and Biomolecular Engineering, North Carolina State University

Background: The thermoacidophilic archaeal order Sulfolobales ($T_{opt} \geq 65°C$, $pH_{opt} \leq 3.5$) has garnered interest from the scientific community for their ability to derive energy from pyritic ores and elemental sulfur to support an autotrophic lifestyle [1]. Sulfur oxidation in particular leverages an energy-rich substrate through multiple energy-conserving steps to support microbial life, and this presents a metabolic engineering opportunity to leverage sulfur oxidation to power CO_2 upcycling into industrially relevant chemicals. However, the only genetically tractable Sulfolobales to date are obligate heterotrophs, so sulfur oxidation capabilities must be engineered into these industrial platforms. The mechanism of sulfur oxidation is complicated by abiotic chemistry from highly reactive reduced inorganic sulfur compound (RISC) intermediates [2], making it difficult to pinpoint the enzymatic requirements for sulfur oxidation. Recent genome sequencing of the Sulfolobales [3] provides a means to assess the necessary components for sulfur oxidation through comparative phenotyping and multi-omics approaches.

Results: The model organism *S. acidocaldarius* (*Saci*) was engineered to oxidize elemental sulfur based on the known sulfur oxidation genes, and its sulfur oxidation performance was benchmarked against native sulfur oxidizers of the Sulfolobales. Scanning electron microscopy was used to verify attachment to the sulfur surface of the engineered *Saci* strain, which has been shown to be necessary for sulfur oxidation to occur. Comparative genomic and transcriptomic analysis of select Sulfolobales was used to identify non-intuitive genes related to the sulfur oxidation, with a specific focus on the unknown mechanism of sulfur oxidation. Free energy of reaction was analyzed for abiotic sulfur chemistries to identify reactions that may play a role in the biological acquisition of elemental sulfur.

Conclusions: Engineered strain *S. acidocaldarius* RK88 demonstrated improved sulfur oxidation, but did not reach levels of native sulfur oxidizers. SEM images demonstrate that *Saci* RK88 does interface with the sulfur surface, but does not appear to form the proximal aggregates observed in native sulfur oxidizers. This aggregation implies that direct surface contact is not required for sulfur oxidation, only proximity to the surface. Comparative multi-omics highlights to key genes necessary for sulfur acquisition. Combining these genes with several key abiotic sulfur reactions, we propose a novel method of sulfur acquisition in the Sulfolobales. Further validation of this mechanism through metabolic reconstruction and comparative flux balance analysis is in progress.

References:
[1] Lewis, AM, *et al*. (2021). The biology of thermoacidophilic archaea from the order Sulfolobales. *FEMS Microbiol. Rev.* **45**(4):1-60.
[2] Willard, DJ and RM Kelly (2021). Intersection of biotic and abiotic sulfur chemistry supporting extreme microbial life in hot acid. *J. Phys. Chem. B.* **125**(20):2543-5257.
[3] Counts, JA, DJ Willard, and RM Kelly (2021). Life in hot acid: a genome-based reassessment of the archaeal order Sulfolobales. *Environ. Microbiol*. **23**(7):3568-3584.

Computational Studies of the Phase Behavior of Dipolar Colloids in the Presence of an External Field

Matthew A. Dorsey [1], Orlin D. Velev [1], Carol K. Hall [1]

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

Background: A new class of engineered materials that interact, assemble, reconfigure, and propel in response to external magnetic and electric fields has been developed by Velev and coworkers [1]. Cubic microparticles with a ferromagnetic-metallic coating on one or two opposing faces retain residual polarization when exposed to an external magnetic field. We use Discontinuous Molecular Dynamics (DMD) simulations to explore the phase behavior of systems of dipolar colloids under various conditions. In our coarse-grained models, the colloidal shape is represented as a series of hard discs bonded together to re-create a rigid geometry, and the dipolar interactions between colloids are represented by opposite charges embedded within the colloidal geometry. Annealing simulations in which the simulation temperature is slowly reduced are used to discover the equilibrium configuration. In recent work, we have explored the phase behavior of large systems of colloidal squares with offset dipoles in the absence of an external field [2]. Additionally, we recently developed a stochastic technique for modeling the effect of an external field on the dynamics of dipolar colloids [3]. We apply these techniques to explore the phase behavior of dipolar colloids in the presence of an external field.

Results: We perform annealing simulations for two colloidal systems in the presence of an external field. First, we extend previous work by Rukowski, et al. [4] to explore how an external field with constant strength and direction shifts assemblies of certain dipolar rods from preference for side-to-side (or anti-parallel) configurations to preference for head-to-tail (or parallel) configurations. Second, we perform annealing simulations in the presence of a constant external field to explore the phase behavior of colloidal squares with dipoles that are offset from the square's center of mass. The nuanced phase behavior of these systems is illustrated with ground-state phase diagrams in the external field strength (H) and reduced density (ϕ) planes.

Conclusions: Our results highlight how the self-assembly of colloidal particles with various degrees of anisotropy can be tuned via application of an external field. Additionally, the technique developed for modeling an external magnetic field is a unique illustration of how stochastic processes can be used in molecular dynamics simulations to model interactions from an external force field. Finally, the computational workflow developed for this research project highlights the advantage of distributed computing for sampling many different conditions with lightweight, coarse-grained simulations.

References:

1. Han K, Shields IV CW, Diwakar NM, Bharti B, López GP, Velev OD. *Sequence-encoded colloidal origami and microbot assemblies from patchy magnetic cubes. Science advances.* 2017 Aug 4;3(8):e1701108.
2. Dorsey MA, Velev OD, Hall CK. *Computational investigation of the phase behavior of colloidal squares with offset magnetic dipoles.* Soft Matter. 2023;19(22):4123-36.
3. Dorsey MA, Hall CK. *Extension of Molecular Dynamics Simulations to Magnetic Ensembles with a Stochastic External Field.* (In-Preparation).
4. Rutkowski DM, Velev OD, Klapp SH, Hall CK. *The effect of charge separation on the phase behavior of dipolar colloidal rods.* Soft Matter. 2016;12(22):4932-43.

Sustainable Conversion of Carbon Dioxide and Shale Gas via a Thermochemical Cyclic Redox Scheme

Sherafghan Iftikhar[1], William Martin[1], Luke Neal[1], and Fanxing Li[1]
Department of Chemical and Biomolecular Engineering, North Carolina State University, 911 Partners Way, Raleigh, North Carolina 27695-7905, United States

Background: Fossil fuels are the primary source of energy in the production of commodity chemicals. As a result, enormous amounts of carbon dioxide (CO_2) are emitted, which severely affects the global climate. Current CO_2 utilization technologies tend to be energy-intensive and have limited CO_2 conversion. Using methane as a co-reactant in a two-step chemical looping scheme, we demonstrated thermochemical reduction of CO_2 with near 100% CO yields, facilitated by the cyclic reduction-oxidation reactions of oxide-based redox catalysts (RCs).[1,2] In addition, experimentally validated computational tools that can effectively narrow down the catalyst design space for CO_2 utilization were also explored.[1]

Results: Based on the optimal equilibrium oxygen partial pressures (PO_2) for CO_2-splitting and CH_4 partial oxidation, density functional theory (DFT)-based materials screening identified a few promising oxide compositions such as $LaNi_{1-x}Fe_xO_3$ and $LaFe_{1-x}Mn_xO_3$ with "x" ranging from 0 to 1. In general, most of the RCs tested in this study exhibited excellent redox performance in terms of syngas yield (85 – 100%) and CO_2 conversion (85 - 100%). $LaFe_{1-x}Mn_xO_3$-based perovskites were found to be highly coke-resistant due to the addition of Mn. In addition, significant improvements in the redox kinetics were realized by impregnating the RCs with 1 wt% ruthenium (Ru), without affecting their redox thermodynamics. We also found that the balance between methane partial oxidation and cracking can be tuned by controlling the Ni-Fe ratio in $LaNi_{1-x}Fe_xO_3$-based redox catalysts, which allows tunable syngas production. Moreover, long-term redox testing over the promising RCs indicated a stable performance with periodic re-activation using air as an oxidant.

Conclusions: The DFT-guided mixed oxide design strategy, which was experimentally validated in this study, can be highly effective in further optimization of the redox catalysts for CO_2 utilization. This study also reports effective approaches to enhance redox kinetics and long-term redox catalyst performance. In addition, various promising catalyst systems for tunable syngas production were also explored. The two-step chemical looping scheme proposed in this study showed a lot of potential to produce syngas, which is a precursor to many industrially important chemicals, with near zero carbon emissions. This represents a great step forward to the sustainable production of commodity chemicals.

References:

1. Wang, X.; Gao, Y.; Krzystowczyk, E.; Iftikhar, S.; Dou, J.; Cai, R.; Wang, H.; Ruan, C.; Ye, S.; Li, F. High-Throughput Oxygen Chemical Potential Engineering of Perovskite Oxides for Chemical Looping Applications. Energy Environ. Sci. 2022, 15 (4), 1512–1528.

2.Iftikhar, S.; Martin, W.; Gao, Y.; Yu, X.; Wang, I.; Wu, Z.; Li, F. LaNixFe1−xO3 as Flexible Oxygen or Carbon Carriers for Tunable Syngas Production and CO2 Utilization.

Enabling Li-S batteries via novel multifunctional dendritic battery separators

Michael J. Petrecca [1], Akhil Shenoy [1], Jaden Leatherman [1], Orlin D. Velev [1], and Peter S. Fedkiw [1]

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

Background: To achieve a sustainable and carbon-neutral society using intermittent energy sources like wind and photovoltaic generators, cost-effective, long-lasting, and reliable methods are essential for storing electrical energy. The presently widely employed Li-ion batteries for load leveling do not present a sustainable and sufficiently efficient solution to this challenge: These batteries use expensive transition metal-oxides (e.g., cobalt) in their positive electrode, and the raw materials are earth-limited and concentrated in countries that are not friendly to U.S. interests. Lithium sulfur (Li-S) batteries are a promising next-generation battery chemistry due to their increased theoretical capacity and energy density compared to Li-ion (1675 vs. 200 mAh/g and 2500 Wh/kg vs. 420 Wh/kg respectively). Li-S cells use sulfur, an earth-abundant element, as the active material in the positive electrode. Sulfur is lower cost and more readily available than the metal oxides used in Li-ion positive electrodes ($32.98 per kg Co vs $0.17 per kg S). The dominant barrier to widespread use of Li-S batteries is the cross-cell shuttling of soluble lithium polysulfides from one electrode to the other through the electrolyte One way in which researchers are combatting this phenomena is by introducing novel types of functional materials into the separator matrix to inhibit the shuttling. Herein, we demonstrate how shear-driven precipitation[1] can be used to develop tailor-made separator composites for the mitigation of polysulfide shuttling in Li-S batteries.

Results: Poly(vinylidene difluoride) (PVDF) soft dendritic colloids (SDCs) are fabricated following previously reported liquid-phase nanofabrication methods[3,4]. Before composite formation, the SDC suspensions are co-dispersed with Al_2O_3 or SiO_2. The battery separators are then produced by vacuum filtering the polymer-ceramic dispersions. The SDC-ceramic composite separators show increased thermal stability, electrolyte uptake, and polysulfide shuttling resistance when compared to commercial porous polyolefin separators. Coin-cell tests in blocking cells and symmetric Li-Li cells also show that the addition of nano-particulate ceramics to the separator matrix increases the ionic conductivity and Li-dendrite suppression capabilities of the SDC-ceramic composites.

Conclusions: This work illustrates the promise of shear-driven precipitation as a manufacturing method for next-generation battery separators. The early results indicate potential for the SDC-formed composites to mitigate polysulfide shuttling and advance towards practical Li-S batteries.

References:

1. Roh, S., Williams, A.H., Bang, R.S., Stoyanov, S.D., Velev, O.D. “Soft dendritic microparticles with unusual adhesion and structuring properties,” *Nature Mater*., 18, 1315- 1320 (2019).
2. Luiso, S.; Williams, A. H.; Petrecca, M. J.; Roh, S.; Velev, O. D.; Fedkiw, P. S.. *J. Electrochem. Soc.* 2021, 168 (2), 020517.
3. Luiso, S.; Petrecca, M. J.; Williams, A. H.; Christopher, J.; Velev, O. D.; Pourdeyhimi, B.; Fedkiw, P.S. *ACS Appl. Polym. Mater*. 2022, 4, 3676-3686

Abstracts for Poster Presentations

Charge-induced Selective Permeability of Viral Capsids by Ionic Molecular Species

Cyrus Cao [1], Eduardo Barberi [1], Seoung Kim [1], Sameera Vellore [1], Stefano Menegatti [1], Orlin D. Velev [1]

1. Dept. of Chemical and Molecular Engineering, North Carolina State University

Background: Ionic species play a crucial role in safeguarding personal care product users against viral infections, including, for example, soaps and sanitizers. While previous studies [1][2][3] have demonstrated the effectiveness of ionic surfactants in combating enveloped viruses such as SARS-COVID, smaller non-enveloped viruses like Norovirus and Poliovirus have proven to be resistant to most existing preventive formulations [4][5]. To address this, we employed the MS2 bacteriophage as a representative model for non-enveloped viruses to assess the antiviral efficacy of different surfactants across a range of pH levels.

Results: By exploring the physiochemical interactions between ionic species and viruses through light scattering and electrophoresis combined with molecular simulations, this research aims to gain deeper insights into the underlying mechanisms involved in virus deactivation. Our research results reveal new details and establish the mechanism by which virus capsids regulate the distribution of ionic substances. Based on the Hendersen-Hasselbalch equation and the capsid protein sequence, our surface charge model suggests that virus capsids have distinct isoelectric points on their interior and exterior surfaces. These surface charges play a pivotal role in determining the virus capsid permeability by ionic substances. When the two surfaces possess opposing charges, it prevents the passage of ionic surfactants, rendering them ineffective as antiviral agents. Conversely, anionic and cationic surfactants exhibit enhanced antiviral effectiveness when the entire capsids carry corresponding positive or negative charges.

Conclusions: The results demonstrate how colloidal theory in combination with data from biological databases enable the evaluation of virus function disruption by ionic species found in personal care products. Overall, our studies lay a foundation for predicting the antiviral effectiveness of formulations based on their ionic and molecular transport properties, thereby prompting means for advancements in the field of antiviral research.

References:

1. Simon M, Veit M, Osterrieder K, Gradzielski M. Surfactants - Compounds for inactivation of SARS-CoV-2 and other enveloped viruses. Curr Opin Colloid Interface Sci. 2021;55:101479.
2. Tsujimura K, Murase H, Bannai H, Nemoto M, Yamanaka T, Kondo T. Efficacy of five commercial disinfectants and one anionic surfactant against equine herpesvirus type 1. J Vet Med Sci. 2015;77(11):1545-1548. doi:10.1292/jvms.15-0030
3. Mertens BS, Velev OD. Characterization and control of surfactant-mediated Norovirus interactions. Soft Matter. 2015;11(44):8621-8631. doi:10.1039/c5sm01778e
4. Liu P, Yuen Y, Hsiao HM, Jaykus LA, Moe C. Effectiveness of liquid soap and hand sanitizer against Norwalk virus on contaminated hands. Appl Environ Microbiol. 2010;76(2):394-399. doi:10.1128/AEM.01729-09
5. Tung G, Macinga D, Arbogast J, Jaykus LA. Efficacy of commonly used disinfectants for inactivation of human noroviruses and their surrogates. J Food Prot. 2013;76(7):1210-1217. doi:10.4315/0362-028X.JFP-12-532

Enabling RNA Uptake in *Caenorhabditis elegans* for Use in Genetic Manipulation

Kaleb Decker [1], Adriana San Miguel [1]
1. Department of Chemical & Biomolecular Engineering

Background: Caenorhabditis elegans, or *C. elegans*, are microscopic nematodes that have been used for several decades for a variety of studies. For example, *C. elegans* are used to investigate the underlying interplay between genes, behavior, phenotype, and function of organisms. Many genetic studies harness CRISPR with accompanying guide RNA (gRNA) to selectively alter portions of the genome. This process is often performed in nematodes using microinjections into the germline of the nematodes. While highly efficient at generating genetic edits, microinjection is time and labor intensive, and is highly dependent on the operator's ability. **Therefore, the primary goal for this project is to circumvent the necessity of microinjections in *C. elegans*, thereby accelerating the experimental process of genetic manipulation for high-throughput experimentation.** Instead of microinjection to supply the gRNA, we propose alternative forms of RNA uptake including feeding RNA and soaking in RNA solution. Worms are already known to uptake double-stranded RNA (dsRNA) for RNA interference (RNAi). However, *C. elegans* typically do not uptake single-stranded RNA (ssRNA), the typical form of gRNA. Therefore, we will focus on two research strategies related to RNA uptake. First, we aim to identify structural characteristics of RNA that facilitate RNA uptake. We will use a variety of sizes and structures of dsRNA and ssRNA to elucidate optimal structures for RNA uptake. There is evidence that shows that *C. elegans* naturally uptake some ssRNA sequences such as the P11 sequence derived from the pathogen *Pseudomonas aeruginosa*. By examining characteristics of P11 such as hairpin, self-folding, and long segments of self-folded RNA, we aim to design ssRNA structures for ssRNA uptake. In the second focus, we genetically alter the RNA uptake mechanisms in *C. elegans* to enable ssRNA uptake. Genetic alterations will be performed using CRISPR-X, which utilizes catalytically dead Cas9 in conjunction with MS2-AIDΔ to generate mutations within a 20-30 bp window. We plan to use CRISPR-X to target domains of *sid-1* and *sid-2*, genes implicated in the transport of dsRNA. By altering these genes, it may be possible to alter the uptake specificity and allow both dsRNA and ssRNA to be uptaken. These two uptake strategies will be used to generate many specific and wide-spread modifications for accelerated examination of the worm genome.

Results: Preliminary results demonstrate that it is possible to feed/soak fluorescent RNA into worms and visualize localization. Upcoming steps include design of RNA structures for uptake experiments, as well as identification of portions of *sid-1* and *sid-2* to alter to induce significant alterations of the transport mechanisms of RNA.

Conclusions: Ultimately, this research will be used to develop a high-throughput genetic analysis pipeline. Upon successful implementation of novel RNA uptake strategies in conjunction with CRISPR/Cas machinery, rapid genetic editing can occur. By designing a host of gRNA sequences, it is possible to target many genes in a single experiment without having to microinject nearly as many worms. Instead, we will soak or feed the worms in RNA solutions that correspond to certain genes. Through this proposed pipeline, we hope to discover key orthologous genes in worms that play a role in the development of neurodegenerative disease in humans. A high-throughput analysis pipeline will accelerate the rate at which we find these key players in neurodegenerative disease.

Recovery of Critical Metals and Rare Earth Elements Using Thermoacidophilic Archaea

MJ H Manesh [1], Dan Willard [1], April Lewis [1], Robert Kelly [1]
Dept. of Chemical and Biomolecular Engineering, North Carolina State University

Background: Bioleaching, aqueous metal extraction from minerals using microorganisms, has emerged as an environmentally friendly alternative to conventional mineral processing, with 15-20% of current copper extraction worldwide attributed to this method [1]. Copper occurs in sulfide minerals, which are refractive in nature. Metal extraction from such ores is energy-consuming due to passivation and metal solubility problems. To overcome these challenges, bioleaching using thermoacidophiles, archaea that thrive in hot acidic environments, have been examined. In this study, thermoacidophilic archaea belonging to the genera *Acidianus*, *Metallosphaera*, *Sulfolobus*, *Sulfuracidifex*, *Saccharalobus*, and *Sulfurisphaera* were used to study the mechanisms of bioleaching of a copper sulfide mineral, chalcopyrite.

Rare earth elements (REEs), including lanthanides, yttrium, and scandium, are being used for a variety of environmentally friendly applications, such as LEDs, wind turbines, and electric vehicles [3]. However, current REE separation processes are environmentally detrimental and energy-intensive, involving toxic organic solvents. The, use of biological ligands has been explored as an alternative for REE separation, with lanmodulin (LanM) from a methylotrophic bacterium being one of the prominent examples of this approach [4]. In this study, two clonal libraries of proteins from a thermoacidophilic archaea, *Saccharolobus solfataricus* (Sso-7d and Sso-6904), are being screened to identify novel binding proteins. These will be immobilized on the surface of magnetic particles, with the protein libraries expressed on yeast surface, and magnetic separation of REE binding proteins on yeast.

Results: A chalcopyrite bioleaching survey of ten thermoacidophilic microorganisms was conducted, and a wide range of copper extraction yields was observed. Redox potential and pH of the cultured were followed over the 21-day testing period. In cultures with high copper extraction, the ratio of ferric iron to total iron was higher, underlying the impact of iron oxidation on bioleaching intensification. SEM images showed difference in the types of layers formed on the mineral after 21 days of bioleaching. Using EDS analysis, elements present on the surface of the mineral after bioleaching was confirmed and used in XRD analysis to identify the potential passivating layers on the mineral after bioleaching.

REEs have been immobilized on phosphate- and carboxyl-modified magnetic, confirmed by XPS and SEM-EDS analysis. The carboxyl-modified magnetic iron oxide nanoparticles will be used for screening protein libraries to find REE binders to be used for chromatographic separation of REEs.

Conclusions: Applications of thermoacidophilic archaea and their proteins in extraction and separation of critical metals was studied. In chalcopyrite bioleaching, complete copper extraction was obtained. In addition, selection procedures are in place to identify proteins with thermoacidophilic origins for separation of REEs.

Investigating the effect of glucose metabolism on stress and differentiation in human cerebral organoids

Gautami R Kelkar [1], Albert J Keung [1].
1. Dept. of Chemical and Biomolecular Engineering, North Carolina State University

Background: Organoids are *in vitro* 3D tissue models derived from human pluripotent stem cells. They capture the complex tissue architecture of human tissues and can be grown in a high-throughput fashion. This scalability makes them a valuable tool for investigating disease etiologies and as drug screening platforms [1]. Organoids are directed to differentiate into particular cell-types by addition of signaling molecules and modifying the nutrients in the culture medium [2,3]. However, these models still face several limitations. For instance, the *in vitro* culture environment, including abundance of nutrients has been found to increase cellular stress and impair differentiation [4]. Particularly, *in vitro* culture systems are known to be hyperglycemic [5,6,7] and studies in murine models have shown that reducing glucose to physiological levels can improve differentiation *in vitro* [8].

Results: Our aim is to investigate the influence of glucose metabolism on oxidative stress and differentiation in human stem cell-derived organoids. Our studies with H1-derived cortical organoids showed that in reduced glycolysis conditions, organoids form large Choroid Plexus (ChP) cysts within two weeks of culture whereas the organoids grown in the typical, high-glucose conditions are limited to cortical cell types. Organoids in altered conditions lacked the neural rosettes that are intrinsic to cortical organoids and were positive for expression of ChP markers TTR, AQP1, and ZO-1 by immunofluorescence analysis. These findings suggest that metabolic substrates can serve as knobs to control differentiation and potentially develop improved model systems.

Conclusions: This study will contribute to the understanding of the interdependence between metabolism and differentiation and help inform strategies for developing new media to generate *in vitro* human organoid models. It has the potential to uncover molecular components and mechanisms that link metabolism to differentiation. Furthermore, this can lead to advanced models for developmental diseases and reveal new therapeutic avenues.

References:

1. Eichmüller, O.L., Knoblich, J.A. Human cerebral organoids — a new tool for clinical neurology research. *Nat Rev Neurol* 18, 661–680 (2022). https://doi.org/10.1038/s41582-022-00723-9
2. Lancaster, M., Knoblich, J. Generation of cerebral organoids from human pluripotent stem cells. *Nat Protoc* 9, 2329–2340 (2014). https://doi.org/10.1038/nprot.2014.158
3. Velasco, S., Kedaigle, A.J., Simmons, S.K. *et al.* Individual brain organoids reproducibly form cell diversity of the human cerebral cortex. *Nature* 570, 523–527 (2019). https://doi.org/10.1038/s41586-019-1289-x
4. Bhaduri, A., Andrews, M.G., Mancia Leon, W. *et al.* Cell stress in cortical organoids impairs molecular subtype specification. *Nature* 578, 142–148 (2020). https://doi.org/10.1038/s41586-020-1962-0

Understanding the relation between neuronal activity, reactive oxygen species (ROS) and oxidative stress resistance using C. elegans

Hrishikesh Mane [1], Adriana San Miguel [1]

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

Background: Neurons are highly energy intensive cells and produce high levels of reactive oxygen species (ROS) as a natural byproduct of mitochondrial respiration. When the cell is incapable of efficiently degrading the ROS produced, it causes oxidative stress. Oxidative stress is said to be involved in the progression of various neurodegenerative diseases and the accumulation of damage due to oxidative stress is also theorized to be a cause of aging. With the proportion of aged individuals and the number of patients suffering from neurodegenerative diseases continuously increasing in the last 50 years, understanding the relationship between neuronal activity, one of the main causes leading to increased ROS and oxidative stress, becomes crucial.

Results: Using increased neuronal activity and reduced stress resistance *C.elegans* mutants like *spr-3, spr-4, slo-1* etc., the available literature hints towards an inverse correlation between the neuronal activity in *C. elegans* and its oxidative stress resistance[1][2]. Thus, in the pursuit of solidifying the above-mentioned inverse correlation, we used putative *C.elegans* loss-of-function mutants like *slo-1* (implications in Alzheimer's disease), *nrx-1* (implications in autism spectrum disorder) and subjected them to paraquat (PQ), a popular oxidant. Compared to wildtype (WT) *C. elegans*, these increased neuronal activity mutants exhibit significantly reduced oxidative stress resistance ($p<0.05$) when cultured at 20℃. Since culture temperature inversely correlates with lifespan in *C.elegans*[3], we tested if the oxidative stress resistance is also affected. All strains show significantly lowered and enhanced oxidative stress resistance (compared to when grown at 20℃) when cultured at a higher (25℃) and lower temperature (15℃), respectively. However, while significant differences in stress resistance between strains exist at 20℃ and 25℃, these differences vanish when the same strains are grown at 15℃. We also measured the neuronal activity of these strains at different temperatures to test if any significant differences with culture temperature exist. The *slo-1* strain showed increased neuronal activity levels (compared to WT) at 20℃ and 25℃ but showed close to WT level neuronal activity at 15℃. We also tried to understand how altering ROS levels affects neuronal activity. We subjected *C. elegans* to an antioxidant (to reduce ROS levels) or an oxidant (to increase ROS levels) in worms and measured their neuronal activity using the aldicarb paralysis assay. Altering the ROS levels using both these techniques reduced neuronal activity of *C. elegans*.

Conclusions: Thus, our preliminary results suggest that the oxidative stress resistance is inversely correlated with culture temperature. However, they also suggest an anomaly in the stress resistance and neuronal activity correlation when *C. elegans* are grown at 15℃. Our results also suggest that altering ROS levels reduces neuronal activity. Future tests are planned to delve further into the anomalous correlation between oxidative stress resistance and lower culture temperatures and understanding the mechanism that alters neuronal activity in response to changing ROS levels

References:

Development of Novel Peptide Ligands for the Purification of AcMNPV Baculovirus

William Smith, Dr. Eduardo Barbieri, Arianna Minzoni, Yuxuan Wu, Laurie Overton, Chris Cummings, Dr. Brandyn Moore, Ryan Kilgore, Dr. Stefano Menegatti
North Carolina State Chemical Engineering Department, North Carolina State Biomedical Engineering Department, North Carolina State Biomanufacturing Training and Education Center (BTEC)

Background: Baculovirus is a tool used by the biopharmaceutical industry for the manufacturing of drug products such as vaccines and gene therapies. Current production-scale purification technology for baculovirus purification is essentially non-existent. Baculovirus has a significant application in the field of gene therapy production, traditional protein production, and mammalian transgenic delivery vectors. By developing a novel peptide for the selective and reversible capture of these delivery vectors, a significant cost reduction in using the baculovirus expression vector system is possible. The only current purification tool against baculovirus is cost prohibitive and limiting the usage of high purity baculovirus within R&D and clinical applications. From a manufacturing perspective, a controlled process with a purified baculovirus product is ideal as it allows for stricter control over the traditional approach of crude infection. In a clinical perspective, the removal of host cell impurities from a baculovirus mammalian expression vector will reduce the likelihood of immune response. There exists the potential for baculovirus to be separated from a complex mixture of biomolecules using the peptide technology.[1]

Results: Preliminary research has shown ~ 80 peptide candidates that have the capability of binding baculovirus particles. These peptide sequences were discovered using the library screening methodology employed by the Menegatti lab. Of these 80 potential candidates, ~ 20 of them have the capability of binding baculovirus based upon a qualitative based selection process. Interestingly, in comparison of the sequence homology specific regions of charge density and hydrophobic properties are present within the sequences. Further details on analytical methods will be discussed, these will include cytometry, HPLC, and qPCR data.

Conclusions: Using the library screening process employed by the Menegatti research group, we have discovered ~ 80 peptide candidates that have the potential for binding baculovirus. Using these peptides, there exists a potential for the development of an affinity chromatography resin to be developed for application in the biomanufacturing industry for the removal or purification of baculovirus particles.

References:

Felberbaum RS. The baculovirus expression vector system: A commercial manufacturing platform for viral vaccines and gene therapy vectors. Biotechnol J. 2015 May;10(5):702-14. doi: 10.1002/biot.201400438. Epub 2015 Mar 20. PMID: 25800821; PMCID: PMC7159335.

Investigating the Mechanisms Underlying Sensory Perception & the Neuronal Contribution to the Oxidative Stress Response

Victoria Yarmey [1][2], Adriana San Miguel [1]

1. Dept. of Chemical and Biomolecular Engineering, North Carolina State University; 2. Dept. of Biomedical Engineering, North Carolina State University

Background: One of the most prominent causes of neurodegenerative diseases is oxidative stress from the buildup of cellular reactive oxygen species (ROS). This causes damage to critical cellular components and may be induced intrinsically or from external stimuli referred to as ROS sources (ROSS). Current research indicates that, in *C. elegans*, sensory neurons have roles in both (1) the extracellular detection of ROSS, and (2) mediating corresponding behavioral responses and stress-resistant gene expression [1-5]. Defining these responses and understanding their underlying mechanisms may prove beneficial for neurodegenerative disease treatment and prevention. This study thus aims to help elucidate the neuronal contribution to the host oxidative stress response (OSR) by defining and quantifying the cell autonomous and non-autonomous OSR in *C. elegans* in response to ROSS.

Results: Neuronal contribution was quantified through avoidance behaviors in response to the ROSS paraquat, juglone, and rotenone. We were able to observe decreased response severity for select chemosensory mutants, with different ROSS requiring specific neuronal subgroups for perception. In examining possible mechanisms responsible for ROSS perception, we found that sensation is affected by internal ROS levels but may not be mediated by typical G protein-couple receptor (GPCR) signaling. Additionally, conditions that elicit neuronal activity do not necessarily prompt host antioxidant expression despite elevated ROS levels.

Conclusions: Specific chemosensory subgroups are responsible for sensing different ROSS, implying a robust and complex system governing the OSR, though perception alone is not responsible for initiating host defense responses. From these results, neuronal perception and involvement is likely related to the ROS generation mechanism in addition to ROS level, as opposed to standard chemosensory reception alone.

References:

1. Bhatla, N., & Horvitz, H. (2015). Light and Hydrogen Peroxide Inhibit C. elegans Feeding through Gustatory Receptor Orthologs and Pharyngeal Neurons. *Neuron 85(4),* P804-818.
2. Gourgou, E., & Chronis, N. (2016). Chemically induced oxidative stress affects ASH neuronal function and behavior in C. elegans. *Scientific Reports 6(38147)*.
3. Li, G., Gong, J., Lei, H., Liu, J., & Xu, X. (2016). Promotion of behavior and neuronal function by reactive oxygen species in C. elegans. *Nature Communications 7(13234)*.
4. Olahova, M., Taylor, S. R., Khazaipoul, S., Wang, J., Morgan, B. A., Matusmoto, K., . . . Veal, E. A. (2008). A redox-sensitive peroxiredoxin that is important for longevity has tissue- and stress-specific roles in stress resistance. *PNAS 105(50), 19839-19844.*
5. Schmitt, C., Schultheis, C., Husson, S. J., Liewald, J. F., & Gottschalk, A. (2012). Specific Expression of Channelrhodopsin-2 in Single Neurons of Caenorhabditis elegans. PLoS One 7(8), e43164.

Kinetic Model for the Thermal Destruction of Perfluorooctanoic Acid

C. C. Murphy [1], H. Ram [1], T. J. Mallo [1], P. R. Westmoreland [1]
1. Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, NC 27606

Background: Per- and polyfluoroalkyl substances (PFAS), one of which is perfluorooctanoic acid (PFOA), form a group of man-made chemicals that have been used for decades in a wide range of industrial and consumer products, such as firefighting foams, non-stick cookware, and waterproofing textiles. PFAS substances are notorious pollutants often referred to as "forever chemicals." These compounds resist natural degradation and possess the ability to dissolve in water. As a result, PFAS compounds bioaccumulate in the environment and in animals. To combat PFAS accumulation, thermal destruction is used to convert fluorine found in PFAS and its intermediates into HF for mineralization.

Results: Molecules, radicals, and transition states were modeled using computational quantum chemistry with Gaussian 16 software. Several combinations of theories and basis sets were evaluated including: B3LYP/6-31G(d,p), M06-2X/6-311+G(d,p), PW6B95-D3(BJ)/def2-TZVP, and ωB97XD/def2- TZVP. Thermochemistry and kinetics were then calculated from these models using statistical mechanics, transition-state theory, and master-equation falloff analysis. It was found that under oxygen-free pyrolysis conditions in plug-flow reactors (PFR), unimolecular pericyclic decomposition routes are predicted to be dominant. In a methane- and oxygen-rich environment in a PFR, abstraction of the carboxylic H by OH or H competes with homolytic breaking of the C-C bonds. H-abstraction rapidly forms perfluoroalkyl radical $+CO_2$. Perfluoroalkyl unzips to perfluoroethylene and perfluoroethyl radicals, or it can form 1H-perfluoroalkane by abstracting an H atom. If the perfluoroalkyl-CF_2COOH bond breaks, it forms perfluoroalkyl and a resonance-stabilized CF_2COOH radical, which then decomposes.

Conclusions: A mechanism for PFOA was developed in promising agreement with recent literature and recent measurements from an EPA pilot incinerator.

A Self-Driving Catalysis Lab for Accelerated Development of Homogeneous Catalysts

J. A. Bennett [1], N. Orouji [1], S. Sadeghi [1], and M. Abolhasani [1]*

1. Department of Chemical and Biomolecular Engineering, North Carolina State University, USA, E-mail: abolhasani@ncsu.edu

Background: Transition metal-based homogeneous catalysts and their associated ligands play a crucial role in various chemical processes such as hydrogenations, carbonylations, oxidations, and coupling reactions [1]. These reactions are integral to both large-scale bulk chemical synthesis and specialized fine chemical and pharmaceutical synthesis, leading to millions of tons per year production [2-4]. Discovering new catalysts can significantly enhance energy efficiency and reduce chemical requirements in reactions and purification. However, ligand discovery in homogeneous catalysis is complex, involving molecular structure and reaction condition optimization. The effectiveness of a ligand varies depending on the transition metal-catalyzed reaction and process conditions, preventing fixed-condition screening strategies. A new approach is needed to explore each ligand's potential across different conditions. This work introduces a closed-loop homogeneous catalysis technology using a flow chemistry platform and self-driving lab principles to accelerate performance benchmarking and development of homogeneous catalysts. The developed self-driving catalysis lab efficiently maps ligand-regioselectivity-yield relationships, showcasing rapid Pareto-front identification.

Results: The self-driving catalysis lab utilizes a modular flow chemistry platform to autonomously explore catalyst/ligand systems for homogeneous hydroformylation of terminal olefins. It seeks to optimize the balance between total aldehyde yield and regioselectivity (linear to branched aldehydes) by employing a dynamic machine learning (ML) modeling and experiment-selection strategy. The ML algorithm constructs a surrogate model using prior experimental data, then uses a Bayesian framework to predict and choose new experimental conditions for automatic testing. The platform's stability and repeatability were validated, ensuring accurate data collection. The self-driving catalysis lab's ability to map the Pareto front—comprehensive reaction outcome ranges—for different ligands was demonstrated. The system's autonomously discovered knowledge was shown to be scalable and transferable to larger-scale batch reactors. The extensive data generated enabled the construction of digital models for each ligand, elucidating how input parameters affect reaction outcomes.

Conclusions: The developed self-driving catalysis lab rapidly identifies ligand performance Pareto-fronts for transition metal-catalyzed homogeneous reactions within a week and using minimal ligand (2 mmol) via autonomous experimentation. Insights into ligand effects are extracted through digital twin modeling and input Shapley feature analysis, offering a powerful method for comprehensively evaluating ligand candidates in the vast chemical structure space.

References:

1. Franke, R., Selent, D. & Börner, A. Applied hydroformylation. *Chemical reviews* **112**, 5675-5732 (2012).
2. Whiteker, G. T. & Cobley, C. J. in *Organometallics as Catalysts in the Fine Chemical Industry* 35-46 (Springer, 2012).
3. Botteghi, C., Paganelli, S., Schionato, A. & Marchetti, M. The asymmetric hydroformylation in the synthesis of pharmaceuticals. *Chirality* **3**, 355-369 (1991).
4. Stanley, G. G. Hydroformylation (OXO) Catalysis. *Kirk-Othmer Encyclopedia of Chemical Technology*, 1-19 (2000).

A Computational Approach to Designing Plastic-Binding Peptides

Michael Bergman [1], Xingqing Xiao [2], and Carol Hall [1]
1. Department of Chemical and Biomolecular Engineering, North Carolina State University; 2. Department of Chemistry, Hainan University

Background: Plastic pollution on the micrometer and nanometer scale, termed micro- and nanoplastics (MNPs), is a pressing environmental issue. Millions of tons of MNPs are in the environment and MNP pollution will continue to accumulate as large plastics break into smaller pieces, intensifying the ongoing plastic pollution problem. Many organisms, including humans, regularly consume MNPs, which can lead to health problems that become more severe as MNP concentration increases. It thus is essential to solve this pernicious environmental problem. Our aim is to computationally design peptides that bind with high affinity to common plastics in order to aid in MNP remediation. Specifically, we are working with collaborators to: (1) develop MNP capture systems comprised of active colloids decorated with our plastic-binding peptide designs, (2) create a MNP detection and characterization platform comprised of our peptides and liquid crystal sensors, and (3) enhance microbial adhesion and degradation of MNPs by expressing the peptides on the surface of microbes engineered to metabolize plastic waste.

Results: We developed the **Pep**tide **P**lastic **B**inding **D**esign (PepPBD) algorithm to design peptides that bind to four of the most common plastics: polyethylene, polypropylene, polystyrene, and PET. PepPBD consists of three main stages. In the first stage, hundreds of thousands of peptide conformations on the plastic surface are sampled to identify the structures that can give rise to relatively strongly interactions between the peptide and plastic. This stage uses a simplified score function to make it computationally tractable. In the second stage, a simulated annealing procedure over sequence and local conformational space is used to maximize peptide-plastic interaction energy for the best conformations identified in stage one. In the third stage, hundreds of thousands of adsorbed conformations of the best amino acid sequences found in stage two are evaluated to account for alternative adsorbed conformations. The top-scoring designs from stage three then undergo additional computational (steered molecular dynamics) and experimental testing (atomic force microscopy and surface plasmon resonance) to characterize their affinity to the target plastic more thoroughly.

Conclusions: Simulation results predict that our best peptide designs for polyethylene have higher affinity than plastic-binding peptides previously found using phage display. These predictions are supported by preliminary experimental results. Computational and experimental testing of designs for polypropylene, polystyrene, and PET are ongoing. Analysis of our best peptide designs show enrichment in amino acids with bulky sidechains and large hydrophobic patches, likely to maximize van der Waals interactions and displace water from a hydrophobic interface. Interestingly, the top peptide designs for different plastics have very similar compositions, suggesting that a single peptide may be capable of capturing many plastic types. We are currently applying machine learning to improve peptide design, and aim to extend PepPBD to design peptides that bind to other materials such as minerals and metals.

MACHINE LEARNING FOR SENSOR DATA INTEGRATION AND QUANTITATIVE EARLY DETECTION OF PLANT DISEASES

Sina Jamalzadegan [1], Giwon Lee [1], Oindrila Hossain [1], Qingshan Wei [1]
1. Dept. of Chemical and Biomolecular Engineering, North Carolina State University

Background: Wearable plant sensors hold tremendous potential for smart agriculture. We report a lower leaf surface-attached multimodal wearable sensor for continuous monitoring of plant physiology by tracking both biochemical and biophysical signals of the plant and its microenvironment. Sensors for detecting volatile organic compounds (VOCs), temperature, and humidity are integrated into a single platform. A machine learning model was developed to analyze multichannel sensor data for quantitative detection of tomato spotted wilt virus (TSWV) as early as 4 days after inoculation. The model also evaluates different sensor combinations for early disease detection and predicts that minimally three sensors are required including the VOC sensors.

Results: To quantitatively assess our multimodal sensors for the early detection of pathogens, an unsupervised machine learning approach based on principal components analysis (PCA) was used to analyze the real-time sensor data. For the demonstration, we used the TSWV inoculation data as an example. The multichannel wearable sensor data from the same plant was first divided into different days (e.g., days 0, 1, 2, 3, etc.). Day 0 data were used as the healthy control and compared to other days. Data from different days were clustered by PCA with reduced data dimensions. Then, the centroid and Euclidean distance between two centroids of clusters (two different days) were calculated. The separation of the clusters was quantitatively assessed by a parameter called "discriminability" (D). According to the discriminability values, a minimum of three sensors is needed for the early detection of TSWV (differentiation from the healthy status). The results suggest that for effective disease detection, the biochemical VOC sensor is probably the most important sensor that is needed in each sensor combination; in addition, the leaf surface humidity sensor works slightly more effectively than the leaf temperature sensor in disease detection.

Conclusions: In this research, we conducted PCA analysis as one of the most common unsupervised machine learning algorithms to reduce the dimensions of multichannel sensor data and also classify the roles of each sensor in combination to find out the best combination candidates to predict plant disease sooner. This data analytics–coupled sensor platform could be used for various applications related to plant health monitoring and crop loss prevention in agricultural settings. To the best of our knowledge, this represents the first report of a multifunctional wearable plant sensor coupled with machine learning data analysis.

References:

1. Lee, G., Hossain, O., Jamalzadegan, S., Liu, Y., Wang, H., Saville, A. C., Shymanovich, T., Paul, R., Rotenberg, D., Whitfield, A. E., Ristaino, J. B., Zhu, Y., & Wei, Q. (2023). Abaxial leaf surface-mounted multimodal wearable sensor for continuous plant physiology monitoring. Science Advances, **9(15)**, eade2232.

Coil to Helix Transitions in Polyelectrolytes

Karthik Sinha [1], Artem Rumyantsev [1]

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

Background: The Coil-to-helix transition is an important phenomenon to understand as it lies at the root of certain neurodegenerative diseases. Moreover, the presence of α helix segments in proteins has a significant impact on the function of the protein and helps in their opening and closing due to the higher rigidity of the α helix structure. In this work, the first step to coming up with a theory that describes the coil-to-helix transition in synthetic polypeptides and proteins is examined. While the previous models are effective at accurately predicting the behavior of proteins with a net neutral charge, where only short-range interactions are substantial, they are not sufficient when it comes to dealing with proteins that have a net nonzero charge. In this case, long-range interactions have a significant impact on the system's behavior, which can not be accounted for by the classical models of the Zimm-Bragg type. In this work, a model single-chain polymer is studied, whose monomers can be either in the random coil state or the alpha helix state for a given set of conditions.

Results: Based on the free energy analysis of the system, it was concluded that, upon polymer ionization, four different scenarios of conformational behavior can take place. These are characterized by the parameter *s* derived from the Zimm and Bragg model. [1] *s* denotes the ease of converting a monomer from a random coil state to the alpha helix state. There are two defining values for s that determine whether the ionization-induced helix-to-coil transition takes place or not. The first is the critical minimal value s_c required to provide the helix formation at a low degree of ionization f. The second value denoted s^* is the threshold, above which the helix-to-coil transition fades away and helical state remains stable for all f. Between the two values, the transition is realized, which can be either direct or reentrant helix-coil-helix transition. Characteristic scaling laws for different conformational regimes are provided.

Conclusions: The Coulomb free energy is crucial in understanding the behavior of helicogenic polyelectrolytes. The polymer in the random coil state can extend itself to lower the Coulomb free energy. The helix state on the other hand, while favorable under certain conditions, cannot extend. Therefore, there is a constant competition between the propensity to form a helix and the Coulomb free energy which ultimately determines what state the system chooses to be at. Although this model provides a simplified representation of the underlying biological problem, it provides important information on how the system can be expected to behave. Further features are to be introduced in the model to provide a more quantitative description of the conformational behavior of ionic polymers capable of coil-helix transition.

References:

1. Zimm, B. H., Bragg, J. K. (1959), Theory of Phase Transition between Helix and random Coil in Polypeptide Chains, *J. Chem. Phys.* 31, 526-535

The Glass Transition in Indomethacin/Sucrose Benzoate Co-Amorphous Drug Delivery Systems

Elaheh A. T. Moghadam, Sindee L. Simon
Dept. of Chemical and Bimolecular Engineering, North Carolina State University

Background: The glass transition temperature (T_g) and related dynamics are investigated for binary miscible mixtures of indomethacin and sucrose benzoate using differential scanning calorimetry. These mixtures are termed co-amorphous glasses, and such materials have been shown to have enhanced water solubility and bioavailability relative to the crystalline forms of active pharmaceutical ingredients. For the co-amorphous glasses studied, the composition-dependent T_g displays negative deviations from expectations for an athermal mixture. However, composition-dependent ΔC_p shows a positive deviation from expectation. The data cannot be described by the Fox equation. The ability of other approaches to describe composition-dependent T_g and ΔC_p will be discussed. In addition, the cooling rate dependence of T_g and the fragility of each mixture is determined in an effort to clarify the relationship between fragility, ease of glass formation, and stability of the glass against crystallization.

Results: All co-amorphous systems exhibited no melting and only a single T_g as indicated by the endothermic step change in heat capacity, indicating that the mixtures are homogenous and single-phase systems. T_g values decrease as the IND composition decreases. The Fox and Gordon-Taylor equations do not describe the data indicating that ideal solution theory is not a good assumption for this system. Moreover, the experimental data for the mixtures lie below the predictions for an ideal solution suggesting that hydrogen bonding is diminished or weakened in the mixtures. The Kwei, Braun Kovacs, and 2-suffix Margules models all do a good job of describing the data, with the 2-suffix Margules being somewhat better. Using the same parameters to fit the models for T_g data predicts a positive deviation in ΔC_p vs. composition. T_g and ΔC_p vs. composition cannot both be described with one set of parameters for the indomethacin/sucrose benzoate system. Additionally, fragility is found to be independent of composition for the indomethacin/sucrose benzoate system. On the other hand, preliminary crystallization studies indicate that indomethacin is the least stable and fastest to crystallize of the systems studied, the co-amorphs have an intermediate crystallization rate, and stability and sucrose benzoate does not crystallize. Thus, for this system, fragility is not a good indicator of glass stability in contrast to other reports. [1]

Conclusions: Indomethacin and sucrose benzoate form co-amorphous glasses. For indomethacin/sucrose benzoate glasses, the composition-dependent T_g and ΔC_p both show a negative deviation from the ideal solution theory. The T_gs in co-amorphous systems can be described by activity coefficient models, including one- and two-suffix Margules. Changes in ΔC_p in indomethacin/sucrose benzoate glasses cannot be described using the model parameters that describe T_g. Thus, there is an inconsistency between the model and the data. Fragility does not seem to predict glass stability in indomethacin/sucrose benzoate. Future work will include crystallization studies and measurement of the absolute heat capacity of co-amorphous samples.

References:

1. M. L. F. Nascimento, L. A. Souza, E. B. Ferreira, and E. D. Zanotto (2005), Can glass stability parameters infer glass forming ability?, J. Non-Crystalline Solids, 351, 3296- 3308.

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

Mesbah Ahmad [1], Darpan Shukla [2], Yong Zhu [2], Orlin D. Velev [1]

1. Dept. of Chemical and Biomolecular Engineering, North Carolina State University; 2. Dept. of Mechanical and Aerospace Engineering, North Carolina State University

Background: Soft stretchable and flexible devices are an emerging class of electronics with a wide range of applications such as robotics [1], medical advancements [2], and defense technologies [3]. However, the rise of these electronics raises new environmental concerns, primarily stemming from the accumulation of electronic waste. The environmental impacts of these technologies can be minimized by the development and integration of sustainable, biodegradable materials. Notably, the selection of biodegradable circuit substrates plays a critical role, given that substrates constitute the bulk weight of these soft electronic devices [4]. Stretchability and flexibility hold vital importance for these substrates, particularly in the context of developing skin-like and biocompatible devices. Chitosan is a natural biodegradable polymer that can be used as a substrate for soft electronics. Through the incorporation of plasticizers like glycerol, the functional attributes of biopolymer films can be greatly enhanced, thereby imparting stretchability and flexibility [5]. Consequently, plasticized chitosan films have a large potential to replace the prevailing synthetic, non-biodegradable films derived from fossil fuels.

Results: Chitosan films were prepared by solution casting method using glycerol as the plasticizer. The mechanical properties of the films at different ratios of the biopolymer and glycerol were characterized. With the increase in glycerol content, the ultimate tensile strength for the films was observed to be less than 2 MPa, and the elongation at break was recorded to be 116%. The thermal stability of the films was investigated using thermogravimetric analysis, which demonstrated that chitosan/glycerol films remain stable at elevated temperatures. The swelling and the weight loss due to leaching in water were also studied to characterize the film's hydrostability. Silver nanowire (AgNW) patterns were printed on the chitosan substrates using the transfer printing method. The biodegradation properties of the printed substrates were investigated, and the study showed that the AgNW-printed chitosan films readily degraded in the presence of enzymes such as lysozyme.

Conclusions: In this work, plasticization of chitosan biopolymers was demonstrated to reduce rigidity and impart stretchability in the films. The outcomes of this work suggest the way for pioneering technologies that can facilitate the manufacture of flexible, extensible, and eco-friendly substrate films, tuned for application in soft electronics. The integration of plasticized biopolymers into electronic circuits and devices constitutes a significant leap forward in the realm of wearable and implantable electronics.

MOF-based hybrid aerogels for enhanced functionality

Vahid Rahmanian , **Muhammed Ziauddin Ahmad Ebrahim**, Seyedamin Razavi , Mai Abdelmigeed, Eduardo Barbieri, Stefano Menegatti , Gregory N. Parsons , Fanxing Li, Tahira Pirzada and Saad A. Khan
Department of Chemical & Biomolecular Engineering, NC State University, Raleigh.

Background: Metal-organic frameworks (MOFs) are porous crystalline substances that belong to a group of coordination polymers and are typically produced in powder form. They have a three-dimensional network structure with exceptionally high surface area and pore volume. MOFs have been extensively researched and have shown potential in applications such as gas storage, separation, and energy storage. Although the use of MOFs in powder form is limited, their applications can be expanded by incorporating them into hybrid composite materials like polymer aerogels that provide a solid host matrix. Aerogels are ultra-light, highly porous materials with low density and large specific surface area. Incorporating MOFs into a porous and interconnected 3D macrostructure can overcome the shortcomings of MOF powders, such as agglomeration, mechanical robustness, and limited accessibility to the pores of MOFs

Results: Nanofibrous aerogels (NFAs) were fabricated through a solid-templating process, utilizing cellulose-silica electrospun nanofibers as the base material. A zinc oxide layer was incorporated into the NFAs, followed by the utilization of a vapor-phase synthesis technique to grow ZIF-8 on the aerogels. The MOF-integrated aerogels displayed remarkable mechanical robustness and enhanced functionality. The ZIF-8 aerogel exhibited a high adsorption rate towards CO_2 due to improved exposure of the active sites within ZIF-8 MOF being loaded on a 3D substrate. The aerogel also demonstrated excellent performance in removing heavy metal, notably copper, achieving a removal efficiency of over 99%. Additionally, the antibacterial property of the hybrid aerogels was also studied which showcased significant reduction in microbial population for both gram-negative and gram-positive bacteria.

Conclusions: This study presents a versatile and one-pot strategy to grow MOFs on (NFAs) utilizing vapor phase deposition and a solvent-free approach. Ultralight and mechanically strong aerogels were fabricated by successfully growing ZIF-8 thereby creating enhanced functionality. The microporosity of ZIF-8 coupled with high specific surface area of NFAs helped in a high CO_2 adsorption capacity. The ZIF-8 also works in synergy with the aerogel matrix to provide a framework with tunable pore size, hierarchical porosity, and abundant functional groups, facilitating strong binding sites for copper. Importantly, the mechanical robustness of the aerogel, withstanding large deformations without collapsing, widens its applications in various fields. In summary, our study highlights the potential of MOF-based hybrid nanofibrous aerogels as sustainable and scalable materials with superior functionality across various domains.

“Moonwalking” active colloidal rollers with organized nanoparticle chains

Abhirup Basu [1], Eric Buchsbaum [1] & Orlin D. Velev [1]

1. Department of Chemical & Biomolecular Engineering, NC State University

Background: Active or self-driven particles represent a unique subset of colloidal particles capable of autonomously extracting energy from their surroundings and using it for their propulsion. Through continuous energy consumption and dissipation, they can generate localized field and flow gradients, independently propelling themselves. In particular, the creation of magnetically responsive colloidal rollers, containing internally embedded and structured components, offers the potential to externally manipulate their macroscopic motion using a magnetic field. This offers distinct advantages compared to alternative self-propulsion methods since magnetic field characteristics can be precisely controlled, altering the particles’s rate and direction of propulsion over time.

Results: We assembled chains of iron oxide nanoparticles (MNPs) inside microdroplets of polydimethylsiloxane (PDMS) precursor by using a static magnetic field. The microdroplets were then crosslinked to form soft PDMS microbeads with embedded aligned nanoparticle structures. These particles demonstrated active rolling motion when subjected to a rotating magnetic field. This rotational motion of the microbeads leads to the forward translational movement in Newtonian fluids and the beads can be propelled backward by reversing the direction of the rotation of the magnets. We found a linear proportionality of the velocity with respect to the frequency of rotation of the magnetic field and with respect to the microbeads size. When immersing these rollers in a shear thinning fluids of increasing viscosity, we registered reduced translation until it reached a static point. As the concentration of the medium increased further, we observed a remarkable new backward “moonwalking” pattern where the translation is opposite to the direction of the rotation of the particles. We hypothesize that this peculiar motion is due to a difference in the shear force on the top and bottom of the particle. Our experimental findings have been supported by COMSOL simulation where we see a fluid shear stress mismatch on the top half of the particle and the bottom half of the particle close to the wall. Finally, at the highest viscosities, the viscous drag overpowers the magnetic torque, and the particle can no longer align with the magnetic field as it wobbles in place.

Conclusions: Our research unveiled a fascinating novel phenomenon about the translation dynamics of rotating colloidal particles within non-Newtonian shear-thinning fluids. It amounts to a new physical principle of active propulsion. This discovery holds the potential to enhance our comprehension of the fundamental principles that could make possible future applications of active rollers in sophisticated biomedical applications.

A Novel System for High-temperature Thermal Energy Storage: Oxide-Molten Salt Composites (OMS)

Hilal Bektas [1], Runxia Cai [1], Xijun Wang [1,2], Fanxing Li [1]

1. Dept. of Chemical and Biomolecular Engineering, North Carolina State University; 2. Dept. of Chemical and Biological Engineering, Northwestern University

Background: While the combustion of fossil fuels is the primary source of greenhouse gas emissions, recovery of waste heat released from the combustion process remains a challenge [1]. The primary obstacle in harnessing industrial waste heat lies in its intermittent nature and aligning the waste heat with the operational requirements of various industrial processes. Therefore, a cost-effective energy storage system that can tailor the properties of waste heat by storing the available energy and releasing it when needed is highly desirable. We propose a novel composite material design called oxide-molten salt composites (OMS) that combines the latent heat from the phase change of eutectic molten salts and the thermochemical energy from the redox reactions of perovskite oxides for ultra-high-capacity thermal energy storage. Conventional molten salt systems suffer from thermal instability and corrosiveness. To address these challenges, our material design limits the adverse interactions of molten salt with the atmosphere and equipment to avoid thermal instability and corrosiveness by filling the pores of perovskites with liquid salt. While perovskite oxides provide support as the exoskeleton, they contribute to the energy storage within a tunable temperature swing owing to their flexible structure and tailorable thermochemical properties.

Results: We optimized the design of perovskite oxides with a high-throughput approach by combining experimental screening with density functional theory-based simulation [2]. We applied thermodynamic-based screening criteria to the simulation results of over 2000 perovskite oxides and selected 61 promising TCES candidates for experimental evaluation. We measured the oxygen capacity and reaction enthalpy of the selected candidates. SCFM1726 achieved the highest energy density of 285 kJ/ kg_{ABO3} in 400 °C/0.2 atm O_2 and 1100 °C/Ar and was chosen as the base material for the composite material optimization. We investigated the compatibility (no reaction) between various perovskite oxides and eutectic salt mixtures via a preliminary screening approach and found 11 compatible combinations among 22 tested. SCFM1726 and a molten salt mixture showed good compatibility and achieved an overall energy density of 565 kJ/kg. Yet, a notable decrease in the heat capacity (~20% kJ/kg) was found due to the thermal loss of the salt during 100 cycles. Meanwhile, $La_xSr_{1-x}FeO_3$ (LSF)-based perovskites were found to have less tendency to react with the same family of salts. Another LSF based composite material showed excellent stability and maintained an overall energy density of 565 kJ/kg over 100 cycles within a 150 °C temperature swing.

Conclusions: We demonstrated that redox-active perovskite oxides and eutectic molten salts can provide a compatible dual-phase structure to offer superior energy storage capacity (> 500 kJ/kg) within a narrow temperature range over long-term.

References:

1. Miró, L.; Gasia, J.; Cabeza, L. F. Thermal Energy Storage (TES) for Industrial Waste Heat (IWH) Recovery: A Review. Appl. Energy 2016, 179, 284–301. https://doi.org/10.1016/j.apenergy.2016.06.147.

2. Cai, R.; Bektas, H.; Wang, X.; McClintock, K.; Teague, L.; Yang, K.; Li, F. Accelerated Perovskite Oxide Development for Thermochemical Energy Storage by a High-Throughput Combinatorial Approach. Adv. Energy Mater. 2023, 2203833.

Surface-initiated ATRP using gelatin-based materials as transfer mediums and reducing agents

Nathanael Brown [1]; Jan Genzer [2]

1. Materials Science and Engineering, North Carolina State University
2. Chemical and Biomolecular Engineering, North Carolina State University

Background: Atom Transfer Radical Polymerization (ATRP) relies on a macroinitiator center with rapidly shifting active and dormant states, which enables controlled polymer growth with low molecular weight dispersity (Đ) and engineered polymer sequences. The metal catalysts driving this reaction require expensive post-synthesis extraction, thus inspiring significant research into minimizing and replacing metal catalyst systems. We investigate using gelatin-based hydrogel (GHs) to reduce metal catalyst use and simplify post-synthesis polymer extractions. Gelatin-based hydrogels exhibit beneficial absorbent and weeping characteristics from a hydrophilic net-like structure of crosslinked polymers. This network permits bulk-like diffusion characteristics when network mesh size is significantly greater than diffusing solutes, thus making hydrogels extremely attractive for applications in controlled solute release [1]. Additionally, native guanidine and carboxylate moieties within GHs permit metal chelation, thus creating a beneficial environment for ATRP [2]. Here, GHs conduct surface-initiated ATRP via the absorption and subsequent weeping of solutions and solutes from the GHs to a surface, creating an active polymerization interface.

Results: We investigate the (1) ability of GHs to absorb solutions containing monomer and solvent, (2) to serve as viable reductive centers for metal catalysts activation from dormant Cu(II) to Cu(I), and (3) conduct surface-initiated ATRP while maintaining low Đ. Due to improved solubility in aqueous media and the homogeneous presence throughout the GHs, Cu(II) was more active in polymerization than Cu(I), indicating reduction behavior within the GHs. This reduction behavior was enhanced when exposed to UV light of 365nm wavelength due to ligand-metal charge transfer (LMCT) reducing ligand-metal complexes and producing stabilized carboxylate radicals [3]. UV analysis reveals an increasing sharp 709 nm peak intensity in solutions containing Cu(I) and a decreasing broad 930 nm peak intensity in solutions containing Cu(II). GHs surface-initiated ATRP resulted in brush lengths up to 161.25 ± 0.739 nm with varying effects of UV exposure due to unwanted initiation within the GHs, creating competing interfacial and bulk polymerization reactions.

Conclusions: GHs exhibit (1) helpful absorption of monomer solutions, (2) the ability to reduce dormant Cu(II) to Cu(I), and (3) active rolls in surface-initiated ATRP. These findings pave the way for alternative methods of conducting ATRP reactions with minimal catalyst concentrations, solvent volumes, and post-polymerization extraction at a small scale.

References:

1. Barros, W. (2019). Solvent self-diffusion dependence on the swelling degree of a hydrogel. *Phys. Rev. E* **99**: 52501
2. Xu, Z., Weng, S., Li, C., Jin, M. & Wan, D. (2020). Dense and robust amino polycarboxylic acid-decorated porous monoliths for eliminating trace Cu (II) or Zn (II) from water. *Colloids Surfaces A* **586**: 124310

Dynamic Exploration of Quantum Dot Synthesis in a Continuous Flow Reactor

Fernando Delgado-Licona[1], Hannah Dickerson [1], Abdulrahman Alsaiari [1], Milad Abolhasani [1]

Dept. of Chemical and Biomolecular Engineering, North Carolina State University

Background: Self-driving labs (SDLs) have emerged as a powerful strategy for accelerating the pace of materials and molecular discovery by 10×-100× compared to the state-of-the-art experimentation techniques. This research acceleration paradigm has been made possible through the integration of disruptive physical and digital technologies such as robotics, reaction miniaturization, and artificial intelligence.[1] Implementations of SDLs that utilize intensified continuous flow strategies in modular microfluidic reactors, *i.e.*, self-driving fluidic labs (SDFLs), have demonstrated to enhance heat and mass transfer rates through an increased surface to volume ratio, shortening startup and shutdown times, lowering reaction time, and decreasing precursor consumption. Despite the growing adoption of SDFLs, their data generation capabilities have been sub-optimal. [2] In response, we present a data-rich method to explore the synthesis parameter space of colloidal quantum dots (QDs). By studying real-time *in-situ* obtained data from dynamic experiments in an intensified fluidic platform, we demonstrate the feasibility of accelerated process-property relationship mapping of cadmium selenide (CdSe) QDs while reducing the raw materials and timescales of traditional steady-state continuous flow experiments.

Results: Real-time transient data obtained from dynamic experiments can accurately approximate (< 1% error) steady state optical features of CdSe QDs, increasing 250× the data-density of automated experimental campaigns, while reducing 2× the processing time and up to 3× the material consumption. High quality continuous synthesis of CdSe QDs was achieved using an intensified reactor geometry exhibiting plug-flow behavior. The reactor consisted of helical sections (1/8" curvature diameter) followed by 90° bends. The flow rate was changed dynamically following a linear ramp controlling the instantaneous residence time of the system.

Conclusions: The intensified modular flow chemistry strategy presented in this work presents an attractive approach for accelerated parameter space exploration of QDs, unleashing the power of continuous flow reactors. Residence time and molar ratios were changed dynamically to accelerate process-property relationship mapping of colloidal QDs while reducing the overall material consumption. Real-time analysis of transient conditions could represent a significant contribution towards optimal utilization of the data generated by SDFLs for autonomous materials discovery. Further technological integrations such as machine-assisted decision making could further accelerate the discovery, development, and manufacturing of higher quality semiconducting nanocrystals for energy, display, and chemical technologies.

References:

1. F. Delgado-Licona, M. Abolhasani, Research Acceleration in Self-Driving Labs: Technological Roadmap toward Accelerated Materials and Molecular Discovery, Advanced Intelligent Systems. 5 (2023) 2200331. https://doi.org/10.1002/aisy.202200331.
2. B.M. Wyvratt, J.P. McMullen, S.T. Grosser, Multidimensional dynamic experiments for data-rich process development of reactions in flow, React. Chem. Eng. 4 (2019) 1637–1645. https://doi.org/10.1039/C9RE00078J.

New modes of active particle propulsion remotely powered by AC fields

Nidhi M. Diwakar [1], Gilad Yossifon [2], Touvia Miloh [2], Orlin D. Velev [1]
1. Dept of Chemical and Biomolecular Engineering, North Carolina State University; 2. School of Mechanical Engineering, University of Tel-Aviv

Background: Active particles are a new class of matter that 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 particle-localized gradient, whether it be physical or chemical. A variety of methods to induce this self-propulsion have been explored, including stimulation by magnetic, electric[1-3], acoustic, optical, biological, and chemical means. Despite these strides, the field of active particles faces the ongoing challenge of using new principles and functionalities. Here we present our work on asymmetric alternating current (AC) field propulsion that grants multiple new degrees of freedom to AC field-driven active particles.

Results: We present our findings on a major new electrohydrodynamic effect, asymmetric field electrophoresis (AFEP), in which spatially uniform, but temporally non-uniform, alternating current (AC) signals drive field-collinear motion of symmetric particles. The results reveal that temporally asymmetric AC fields lead to an active particle propulsion through induced uneven ionic polarization of the ionic charge layer. The reversal of the AC signal symmetry results in a reversal of particle direction of motion without a change in speed. We characterize the particle velocity as a function of field strength, frequency, and signal asymmetry. The experimental electrophoretic findings are supported by theoretical and numerical models of the effect of the asymmetric sawtooth wave signal, considering the resulting asymmetric ionic concentration-polarization effect due to surface conductance. AFEP opens multiple opportunties for electrohydrodynamic control of particle motion and active propulsion. The direction of particle migration exhibits a crossover in the low frequency domain, which is dependent on particle size and can be harnessed for simple and highly efficient particle sorting and on-chip separations.

Conclusions: To our knowledge, this is the first investigation characterizing the behavior of particles with respect to the degree of an AC field time-based asymmetry. It shows that the motility of these particles is a result of local ionic concentration-polarization and particle-centered dissipative flows. The motility driven by particle-induced gradients is in agreement with the definition of "active" or "self-propelling" systems. Thus, we envision that this new effect could add to the toolbox of AC EHD effects, by enabling another convenient way to control and manipulate AC field-driven active particle systems.

References:

1. S. Gangwal, O. J. Cayre, M. Z. Bazant and O. D. Velev, Phys. Rev. Lett., 100, 058302 (2008). Induced-Charge Electrophoresis of Metallodielectric Particles.
2. C. W. Shields, K. Han, F. Ma, T. Miloh, G. Yossifon and O. D. Velev, Adv. Funct. Mater., 28, 1803465 (2018). Supercolloidal Spinners: Complex Active Particles for Electrically Powered and Switchable Rotation.
3. N. M. Diwakar, G. Kunti, T. Miloh, G. Yossifon, and O. D. Velev, AC Electrohydrodynamic Propulsion and Rotation of Active Particles of Engineered Shape and Asymmetry, Curr. Opin. Colloid In. 59, 101586 (2022).

A new method for efficient microplastic remediation utilizing self-propelling and self-dispersing active microcleaners

Haeleen Hong [1], Rachel S. Bang [1], Lucille Verster [1], Orlin D. Velev [1]

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

Background: Given the enduring presence and harmful effects of microplastics in various aquatic ecosystems, the removal of these particles has emerged as a critical environmental challenge. Traditional approaches to water treatment, such as filtration and centrifugation, are not viable solutions for dealing with the vast quantities of natural water due to their exorbitant expenses, limited processing capacity, and adverse impacts on aquatic ecosystems.

Results: We propose a novel remediation approach centered around active microcleaners designed to effectively eliminate microplastic particles within aquatic environments. These active microcleaners achieve this by autonomously navigating through the water and possessing a morphology optimized for highly efficient particle capture. Our active cleaners consist of dehydrated and concentrated soft dendritic colloids (SDC) characterized by an intricately branched hierarchical structure. [1]. This structural complexity enables them to adhere to microplastic particles via van der Waals forces. Notably, the microcleaners are made of chitosan, a sustainable biomaterial, and their clustered particles are infused with a fatty acid that generates surface tension gradients, empowering them to autonomously propel across the water's surface through the Marangoni effect. Our investigations have demonstrated the remarkable capabilities of these active cleaners. They can traverse substantial distances and disperse over large water areas before undergoing rehydration, descending, and efficiently capturing microplastic particles, substantially amplifying their remediation efficiency. Our findings underscore that the propulsion of these microcleaners is contingent on factors such as surface tension, the solubility of the fatty acid, and the area covered during traversal. Notably, when infuse with with just 0.1 µl of eugenol, these active cleaners can sustain propulsion for over 400 s, covering distances exceeding 8 m at speeds exceeding 300 mm/s. During the rehydration process, the rapid propulsion engenders fluid shear, facilitating the restoration of the original highly branched dendrimer structure of the SDC structure and enhancing its efficacy in capturing microplastics.

Conclusions: The active self-propelling and self-dispersing dendritic colloid system that we have designed holds promise for efficiently addressing microplastic pollution across diverse aquatic environments, including saline seawater conditions. We expect that this research could pave the way for a novel approach to microplastic remediation in real aquatic environments, offering cost-effectiveness, reduced energy demands, and biocompatibility as key advantages.

References:

1. Roh, S., Williams, A. H., Bang, R. S., Stoyanov, S. D., & Velev, O. D. (2019). Soft dendritic microparticles with unusual adhesion and structuring properties. *Nature Materials,* 18, 1315-1320.

Thermal Properties of Liquid Crystals

Sahel Mohammadkhah, Sindee. L. Simon
Dept. of Chemical and Biomolecular Engineering at North Carolina State University

Background: Liquid crystals are unique materials that exhibit properties of both solids and liquids. Thermotropic liquid crystals, in particular, undergo phase transitions with increased ordering as temperature decreases from the isotropic liquid phase to various liquid crystal phases, which may include nematic, cholesteric, and smectic phases.[1,2,3] In addition to common applications of liquid crystals, these materials can be used for calibration of differential scanning calorimetry (DSC) on cooling due to the fact that liquid crystal transitions do not typically display supercooling behavior and, hence, do not show hysteresis in their transitions. [2,4-7] Two common liquid crystals for this purpose are N-(4-n-octyloxy-2-hydroxybenzal)-4'-n-butylaniline (LC-l), and (+)-(4-(2'-methylbutyl)phenyl-4'-n octylbiphenyl-4-carboxylate) (CE-8).[6] Here, we investigate the thermal properties of these two liquid crystals, LC-1 and CE-8, using fast scanning calorimetry (Flash DSC) to gain a more comprehensive understanding of their thermophysical properties.

Results: Fast-scanning calorimetry experiments were conducted on LC-1, and CE-8 at temperature range of -95°-150°C with the heating and cooling rate of 1000 K/s using the Mettler Toledo Flash DSC. Preliminary findings revealed a possible glass transition at -55°C and -75°C, for LC-1 and CE-8, respectively, which have not previously been reported by any conventional DSC studies due to the ability of the Fash DSC to apply faster cooling and heating rates. Moreover, for both samples the some of the observed liquid crystalline mesophase transitions were consistent with the conventional DSC results reported in the literature, including the smectic to nematic and the nematic to isotropic transitions [5]. However, CE-8 showed a new presumably LC transition below melting point by passing crystallization. Applying cooling rates in the range of 10,000 to 0.01 K/s on LC-1 and increasing the scanning rate resulted in the observed glass transition. This finding provides confirmation as to why glass transition had not been reported using conventional DSC data.. Also, based on faster scanning rates, a potential cold crystallization process was observed at approximately 20°C, a phenomenon that has not been previously reported in conventional DSC analyses. Investigating the kinetics of this crystallization and understanding the associated glass transition remains a subject of interest for future research.

Conclusions: Liquid crystals with good thermal stability and multiple stable phase transitions are valuable for a wide range of applications. The results of the fast-scanning calorimetry experiments on LC-1 and CE-8 align with the conventional DSC data. Additionally, the faster cooling rate enabled the observation of glass transitions and new transitions in these two materials which are our future research interests.

Acknowledgment: Dr. J. D. Menczel for providing liquid crystal samples for us.

References:

1. Paul Ukleja (2003), Encyclopedia of Physical Science and Technology (Third Edition), 717-739
2. A. D. Campo etal. (2002), Macromol. Chem. Phys., 203, 2508–2515.
3. J. D. Menczel (2011), J Therm Anal Calorim, 106, 7–24.
4. J. D. Menczel, T. M. Leslie (1990), Thermochimica Acta, 166, 309-317.
5. M. Chen etal. (2011) Thermochimica Acta 526 (2011) 58– 64.
6. J. D. Menczel, T. M. Leslie (1993), Journal of Thermal Analysis, 40, 957-970.
7. S. Neuenfeld, C. Schick (2006), Thermochimica Acta, 446, 55–65.

A Material-Efficient Materials Acceleration Platform for Fast-Tracked Exploration of Colloidal Quantum Dots

Nikolai Mukhin[1], Zachary Dubinsky[1], Milad Abolhasani[1]

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

Background: In a world of rapid urbanization and continuous innovation, the escalation of pressing global concerns such as pandemics and climate change invokes immediate attention and resolution. A promising research area to deescalate these pressing issues is with the materials discovery and formulation. Specifically, new emerging materials have been used in various renewable energy technologies such as solar cells to help minimize the carbon emissions in our atmosphere[1]. Current conventional research methods such as manual Edisonian approaches can prove to be time, cost, and material expensive. In the past five years, a new research paradigm for materials discovery and optimization has emerged, known as self-driving labs (SDLs)[2]. SDLs offer a powerful means of expediting the discovery and development of new materials. A class of materials that SDLs can take advantage of are metal halide perovskite (MHP) quantum dots (QDs). In the past decade, MHP QDs have emerged as a highly promising class of semiconducting materials due to their high photoluminescence quantum yield (PLQY), and narrow emission linewidth for energy harvesting devices and displays[3]. Conventional MHP QD synthesis are performed in batch reactors with high chemical consumption and waste generation (~ 6 mL to 100 mL/experiment). Flow chemistry is an alternative approach for MHP QD synthesis, and has shown a lot of promise due to reproducible heat and mass transfer rates, facile *in-situ* QD characterization, and lower material consumption[4].

Results: In this work, we present a material-efficient material acceleration platform (MAP) for rapid exploration of high-dimensional experimental space of colloidal QDs. The developed MAP utilizes a modular flow chemistry strategy equipped with a single-droplet flow reactor for controlled QD synthesis. The single-droplet MAP enables automated access to QD synthesis inputs such as the residence time, temperature, and the ratios of precursors for each individual reactive droplet. The first set of experiments performed was a reproducibility test of the developed MAP. A set of 5 replicate single droplets were sampled out of the same composition at the same input parameters. Over a set of 4 different input conditions and 20 droplets, the test showed to have reproducible droplets with a percent error of less than 3%. Next, the single-droplet MAP was employed for rapid experimental parameter space mapping of MHP QDs.

Conclusions: The material-efficient MAP demonstrated reproducible synthesis of MHP QDs while using 1000x and 100x lower chemicals than batch and continuous flow reactors, respectively. The next steps will include a partial grid search and autonomous Pareto-front mapping of the MHP QD synthesis space. With the integration of machine learning and Bayesian optimization, the PLQY of the in-flow synthesis MHP QDs will be optimized for a target peak emission wavelength while minimizing the emission linewidth.

References:

(1) Wang, J.; Che, Y.; Duan, Y.; Liu, Z.; Yang, S.; Xu, D.; Fang, Z.; Lei, X.; Li, Y.; Liu, S. (Frank). 21.15%-Efficiency and Stable γ -CsPbI3 Perovskite Solar Cells Enabled by an Acyloin Ligand. *Adv. Mater.* **2023**

(2) Abolhasani, M.; Kumacheva, E. The Rise of Self-Driving Labs in Chemical and Materials Sciences. *Nat. Synth.* **2023**.

(3) Lignos, I.; Stavrakis, S.; Nedelcu, G.; Protesescu, L.; deMello, A. J.; Kovalenko, M. V. Synthesis of Cesium Lead Halide Perovskite Nanocrystals in a Droplet-Based Microfluidic Platform: Fast Parametric Space Mapping. *Nano Lett.* **2016**, *16* (3), 1869–1877. https://doi.org/10.1021/acs.nanolett.5b04981.

(4) Antami, K.; Bateni, F.; Ramezani, M.; Hauke, C. E.; Castellano, F. N.; Abolhasani, M. CsPbI $_3$ Nanocrystals Go with the Flow: From Formation Mechanism to Continuous Nanomanufacturing. *Adv. Funct. Mater.* **2022**, *32* (6), 2108687. https://doi.org/10.1002/adfm.202108687.

Effect of Surface Coatings on Biodegradability and Functional Properties of Pure and Blended Biopolymer Substrates

Anicah S. O'Brien [1], Dr. Saad A. Khan [1], Dr. Morton Barlaz [2]

1. Chemical & Biomolecular Engineering, North Carolina State University; 2. Civil, Construction, & Environmental Engineering, North Carolina State University

Background: The excessive use of synthetic, single-use plastics has resulted in environmental concerns regarding the end-of-life management of such products. Biodegradable polymers, such as polylactic acid (PLA) and polybutylene succinate (PBS), have been promoted as a solution as they can be transformed into carbon dioxide, methane, and water by specific microbial populations [1]. However, these polymers require modification to achieve desirable functional properties. For example, PLA has high brittleness and is often blended with other biopolymers to impart flexibility [1]. For use in hygiene products as a nonwoven top sheet, surface modification via surfactant coating is required to impart hydrophilicity. The impacts of blending and surface modification on biodegradability of these polymers have not been investigated in the literature. To encapsulate all possible end-of-life scenarios, studying both aerobic and anaerobic biodegradation is critical. Finally, the findings from this project will contribute to the development of sustainable plastic materials and a circular economy.

Results: Test methods for studying both aerobic and anaerobic biodegradation of various polymers have been fully developed. Preliminary data show that the developed aerobic test is an accurate method for analyzing evolved carbon dioxide over time. The degradation media for the aerobic test was chosen as mature compost derived from food and paper waste. Carbon dioxide output by the compost has been quantified and the microbial population is ensured to be active, as shown by near complete cellulose degradation. To study anaerobic biodegradation, evolved methane is quantified. The microbial population is derived from landfill waste. This method is accurate for measuring anaerobic biodegradation by quantifying evolved methane.

Conclusions: The developed methods for measuring biodegradation will be critical for understanding how various modifications impact polymer biodegradation. By studying both composting and anaerobic biodegradation, we can assess how the material will behave in multiple end-of-life scenarios. The knowledge gathered will aid in the development of biodegradable plastics, thus contributing to a more sustainable and circular world.

References:

1.Ghosh, Koushik, and Brad H. Jones (2021). Roadmap to Biodegradable Plastics-Current State and Research Needs. *ACS Sustainable Chem. Eng.,* **9:** 6170-6187.

Autonomous Nanomanufacturing of Lead-Free Metal Halide Perovskite Nanocrystals Using a Self-Driving Fluidic Lab

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

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

Background: Metal halide perovskite (MHP) nanocrystals (NCs) have been of great interest in photonic devices and renewable energy technologies due to their size- and composition-tunable optical properties, high photoluminescence quantum yield (PLQY), and facile solution-phase synthesis and processing. Despite the intriguing properties of MHP NCs, their adoption by printed technologies is greatly hampered by the lead toxicity. Recently, cesium copper halide perovskite NCs with narrow size distributions and tunable emissions have emerged as a promising lead-free MHP NC candidate. [1, 2, 3] Among copper-based MHP NCs, cesium copper iodide ($Cs_3Cu_2I_5$) exhibits a high air stability and a pure orthorhombic crystal structure, where tetrahedral [CuI_4] and trigonal [CuI_3] units are edge-shared to form [Cu_2I_5] clusters that are isolated by cesium cations. [3] Despite the successful synthesis of $Cs_3Cu_2I_5$ NCs, the fast formation kinetics of these NCs could result in batch-to-batch variations, which complicates their fundamental and applied studies.

Results: Herein, we report an active learning (AL)-guided flow chemistry platform to autonomously synthesize $Cs_3Cu_2I_5$ NCs with the desired optical and optoelectronic properties. Utilizing the process automation mode of the developed flow chemistry platform, we investigate the effects of precursors concentration, ligands population, reaction time, and temperature on the optical properties of the in-flow synthesized $Cs_3Cu_2I_5$ NCs. Utilizing the AL-guided Bayesian optimization (BO) framework, we demonstrate the unique potential of the developed self-driving fluidic lab (SDFL) for accelerated parameter space mapping and on-demand synthesis of rapidly optimized $Cs_3Cu_2I_5$ NCs with minimum experimental cost.

Conclusions: In summary, $Cs_3Cu_2I_5$ 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 and mechanistic studies 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.

References:

1. Li, Y.; Vashishtha, P.; Zhou, Z.; Li, Z.; Shivarudraiah, S. B.; Ma, C.; Liu, J.; Wong, K. S.; Su, H.; Halpert, J. E. Room Temperature Synthesis of Stable, Printable $Cs_3 Cu_2 X_5$ (X = I, Br/I, Br, Br/Cl, Cl) Colloidal Nanocrystals with Near-Unity Quantum Yield Green Emitters (X = Cl). *Chem. Mater.* **2020**, *32* (13), 5515–5524. https://doi.org/10.1021/acs.chemmater.0c00280.
2. Luo, Z.; Li, Q.; Zhang, L.; Wu, X.; Tan, L.; Zou, C.; Liu, Y.; Quan, Z. 0D $Cs_3 Cu_2 X_5$ (X = I, Br, and Cl) Nanocrystals: Colloidal Syntheses and Optical Properties. *Small* **2020**, *16* (3), 1905226. https://doi.org/10.1002/smll.201905226.
3. Lu, Y.; Fang, S.; Li, G.; Li, L. Optimal Colloidal Synthesis and Quality Judgment of Low-Dimensional $Cs_3Cu_2Cl_5$ Nanocrystals with Efficient Green Emission. *J. Alloys Compd.* **2022**, *903*, 163924. https://doi.org/10.1016/j.jallcom.2022.163924.

Impact of Nanoparticle Reinforcement on Polysulfone

Nazanin Shakoury [1], Gregory B. McKenna [1]
1. Dept. of Chemical and Biomolecular Engineering, North Carolina State University

Background: Polysulfone (PSF) is among the few polymers that have a weak β-relaxation and a strong γ-relaxation[1]. These secondary transitions are associated with properties such as elongation and impact strength thus, including fillers in the polymer matrix has the potential for plasticization, reinforcement, or antiplasticization (fortification) by interaction with the β- or γ-relaxations[2]. There are different studies investigating the effect of nanoparticles on the sub-glass relaxations as well as on the glass transition temperature (T_g), indicating that both negative and positive changes in T_g are possible[3],[4]. In this research, we investigate the impact of Al_2O_3 and SiO_2 nanoparticles on the thermal behavior and secondary loss transitions of PSF expecting that the interactions of the nano-sized alumina and silica and PSF can lead to different phenomena using two different methods of sample preparation. Strong attractive interactions between nanoparticles and the host polymer provide the possibility of antiplasticization and reinforcement while plasticization is the outcome of a weak interaction between the filler and polymer[5]. Furthermore, confinement effects on the matrix due to the near neighbor spacing of the nanoparticle dispersions also can impact the polymer dynamics[6].

Results: Preliminary results suggest that the Al_2O_3 and SiO_2 nanoparticles have little impact on the glass transition temperature of the polysulfone for particle concentrations from 1% to 10% alumina, all concentrations of the nanoparticles showed virtually a small increase in T_g (except the 1%). Further work is ongoing to determine the origins of the effect should it be reproducible.

Conclusions: In summary, there is a weak increase in the glass transition temperature (T_g) when the concentration of Al_2O_3 and SiO_2 nanoparticles is increased. This observation suggests a low level of interaction between the nanoparticles and the polymer, hinting at the potential benefits of using nanoparticles with modified surfaces to enhance functionality. Additionally, it was observed that the sensitivity of polymer nanocomposites to the method of preparation, particularly in terms of visual dispersion, is noteworthy. This sensitivity may be attributed to the molecular weight degradation of the polymer during sonication in one of the preparation methods.

References:
1. J. R. Fried, A. Letton, and W. J. Welsh (1990). Polym., “Secondary relaxation processes in bisphenol-A polysulphone,” no. 6: 1032–1037.
2. L. M. Robeson and J. A. Faucher (1969). J. Polym. Sci. [B], “Secondary loss transitions in antiplasticized polymers,” no. 1: 35–40.
3. A. Yim, R. S. Chahal, and L. E. S. Pierre (1973). J. Colloid Interface Sci., “The effect of polymer—filler interaction energy on the T′g of filled polymers,” no. 3: 583–590.
4. B. J. Ash, R. W. Siegel, and L. S. Schadler (2005) J. Polym. Sci. Part B: Polym. Phys., “Glass-transition temperature behavior of alumina/PMMA nanocomposites” no. 1: 114–114.
5. A. C. Comer, A. L. Heilman, and D. S. Kalika (2010). Polymer, “Dynamic relaxation characteristics of polymer nanocomposites based on poly (ether imide) and poly (methyl methacrylate),” no. 22: 5245–5254.
6. M. Alcoutlabi and G.B. McKenna (2005). J. Phys.: Condensed Matter, “Effects of Confinement on Material Behaviour at the Nanometre Size Scale,” no.17: R461-R524.

The Kinetics of Crystallization and the Rigid Amorphous Fraction of Poly(L-lactide)

Logan Williams, Dr. Sindee Simon
Dept. of Chemical and Biomolecular Engineering, North Carolina State University

Background: Polymers are essential components of modern society with applications in various fields ranging from the medical sector to automobile manufacturing. The properties of semicrystalline polymers depend strongly on their morphology and the amount of crystal fraction and amorphous fraction, composed of MAF and RAF. The MAF is the mobile amorphous phase, commonly referred to as the bulk of the amorphous phase. The RAF (rigid amorphous fraction) is a region of amorphous material that is in close proximity with the crystal lattice, thereby limiting its mobility. The RAF is believed to have its own properties, such as a unique glass transition temperature, that influences the properties of the bulk material [1]. In this work, we investigate Poly(L-lactide) (PLLA), a biodegradable polymer of interest due to the ability to easily manipulate its RAF content. In particular, the kinetics of crystallization and the influence of time and temperature on the formation of RAF is studied using differential scanning calorimetry (DSC) and Flash DSC.

Results: DSC was used to obtain a step change in the heat capacity (ΔCp) value for a fully amorphous sample having no crystallinity and therefore no RAF. This value was used to calculate the sample mass for Flash DSC. Samples were allowed to undergo melt crystallization as a function of temperature and time. The crystallinity and ΔCp for all experiments was determined, and RAF was calculated to range from 0% to 16.5%. A modified Avrami model (the Hillier Model) was used to calculate the Avrami exponents (n) and crystallization rate constants (k).

Conclusions: The calculated Avrami exponents reveal crystallite geometry to be that of a spherulite, with interface-controlled nucleation. The crystallization versus time graphs and the Avrami rate constants both confirm relatively fast crystallization rates, as expected for our samples having a relatively low molecular weight (M_n = 25,000 g mol^{-1}). The RAF content (X_{RAF}) is calculated and plotted against crystallization time and temperature, with a maximum RAF content of ~16.5% achieved after only 110 seconds of isothermal holding at 97°C. Future work will examine the effect of physical aging on the rigid amorphous fraction. We will also perform further measurements to determine the glass transition temperature of the RAF.

References:

1. Righetti, Maria et al. (2021). Temperature dependence of the rigid amorphous fraction of poly(butylene succinate). *RSC Adv.,* **11**, 25731.

Wearable Ionotronic Tactile Sensors from Sustainable Homocomposite Hydrogels

Pedro Henrique Wink Reis [1], Haeleen Hong [1], Orlin D. Velev [1], Lilian Hsiao [1]
1. Dept. of Chemical and Biomolecular Engineering, North Carolina State University

Background: The accelerated development and use of wearable human-machine interfaces require the development of soft and stretchable sensors and tactile arrays. Previous scientific studies have leveraged the ionotronic effects exhibited by ionic hydrogels to assemble soft tactile sensors [1-3]. However, the hydrogel-based tactile sensors developed so far often rely on nonsustainable materials and complex chemistry [2,3]. In this study, we report an inexpensive, biocompatible, transparent, and 100% biodegradable soft tactile sensing prototype suitable for wearable applications. It consists of a homocomposite hydrogel composed of sodium alginate reinforced by alginate soft dendritic colloids (SDCs) [4]. The incorporation of alginate SDCs into the hydrogel improves its mechanical properties, ionic response, and enables it to be 3D printed, resulting in a homocomposite material with unique properties and excellent shape control [4].

Results: Electromechanical experiments were performed by measuring the generated voltage spikes concurrently with the changes in resistance experienced by the material under compressive strain at different strains, strain rates, and locations along the length of a hydrogel slab. The compression experiments were performed with an Instron instrument and the electric responses were recorded with a BioLogic potentiostat. In this study, we show that the voltage signal amplitude is a function of the applied stress. We also show that the signal and amplitude of the generated voltage change with the indentation position along the gel length. Additionally, we demonstrate that the addition of SDCs to alginate hydrogels increases its ionotronic effects.

Conclusions: This study shows that the electromechanical strain ionic response of alginate hydrogels reinforced with SDCs can provide information about the applied indentation stress and its position. We demonstrate that higher stresses result in larger voltage peaks and that the sign of these voltage peaks is dependent on the indentation position relative to the electrodes. This allows to precisely measure the touch position, force and rate. We also show that SDCs contribute to the sensitivity of the hydrogel sensor by increasing the voltage response. These results demonstrate that alginate homocomposite hydrogels are an efficient sustainable medium for applications in wearable tactile sensing.

References:

1. Dobashi, Y.; Yao, D.; Petel, Y.; Nguyen, T. N.; Sarwar, M. S.; Thabet, Y.; Ng, C. L. W.; Scabeni Glitz, E.; Nguyen, G. T. M.; Plesse, C.; Vidal, F.; Michal, C. A.; Madden, J. D. W. Piezoionic Mechanoreceptors: Force-Induced Current Generation in Hydrogels. Science 2022, 376 (6592), 502–507.
2. Odent, J.; Baleine, N.; Biard, V.; Dobashi, Y.; Vancaeyzeele, C.; Nguyen, G. T. M.; Madden, J. D. W.; Plesse, C.; Raquez, J.-M. 3D-Printed Stacked Ionic Assemblies for Iontronic Touch Sensors. Adv. Funct. Mater. 2023, 33 (3), 2210485.
3. Boahen, E. K.; Pan, B.; Kweon, H.; Kim, J. S.; Choi, H.; Kong, Z.; Kim, D. J.; Zhu, J.; Ying, W. B.; Lee, K. J.; Kim, D. H. Ultrafast, Autonomous Self-Healable Iontronic Skin Exhibiting Piezo-Ionic Dynamics. Nat. Commun. 2022, 13 (1), 7699.
4. Williams, A. H.; Roh, S.; Jacob, A. R.; Stoyanov, S. D.; Hsiao, L.; Velev, O. D. Printable Homocomposite Hydrogels with Synergistically Reinforced Molecular-Colloidal Networks. Nat. Commun. 2021, 12 (1), 2834.

Data-Driven Synthesis of Metal Halide Perovskite Nanocrystals with an Intelligent Multi-Robotic Platform

Jinge Xu[1], Fazel Bateni[1], Hicham Moran[1], Milad Abolhasani[1]

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

Background: Recently, all-inorganic Metal halide perovskite (MHP) quantum dots (QDs) have emerged as a highly promising class of semiconducting nanomaterials for various solution-processed photonic devices. These quantum-confined nanocrystals exhibit unique optical properties that can be precisely engineered by altering their composition, shape, size, and geometry. The surface ligation of MHP QDs relies on an acid-base equilibrium reaction, which is commonly utilized not only to provide colloidal stability in organic solvents but also to tune their optical properties. The use of various organic acids as surface capping ligands results in distinct growth pathways and thereby different QD morphologies. Consequently, the optical characteristics of MHP QDs are strongly influenced by both the ligand structure (discrete parameter) and the reaction conditions (continuous parameters). The multidimensional nature of this parameter space makes it extremely challenging to comprehensively explore. Traditional synthesis methods for MHP QDs, similar to other colloidal QDs, are time-consuming, material-intensive, and laborious, relying on manual flask-based techniques. The manual nature of these methods, along with the interdependent reaction and processing parameters in colloidal QD synthesis, hinders the discovery of optimal formulations and fundamental understanding of MHP QDs.

Results: In this work, we have developed and deployed a multi-robot self-driving lab (SDL) for accelerated QD synthesis and development research. The developed SDL enables systematic investigation of the effects of ligand structure and precursor concentrations on the photon-conversion efficiency, nanocrystal size uniformity, and bandgaps of MHP QDs. Next, we utilized the developed multi-robot SDL to conduct multiple autonomous experimentation campaigns to rapidly discover the pareto-front of MHP QDs optical properties for various capping ligands.

Conclusions: We overcame challenges of conventional QD research by investigating the science and engineering of a modular autonomous robotic experimentation platform. We established a closed-loop QD synthesis and development strategy by integrating a modular robotic experimentation platform with data-driven modeling and experiment-selection algorithms. The developed SDL accelerated mapping the optical properties of MHP QDs to the ligand structures and synthesis conditions and understanding the underlying role of ligand structure on the shape, morphology, and optical properties of MHP QDs. The SDL-generated knowledge will enable on-demand synthesis of MHP QDs with optimal optical properties for the next generation energy and display technologies.

References:

1.Abolhasani, M. and E. Kumacheva. The rise of self-driving labs in chemical and materials sciences. Nature Synthesis, 2023. 2(6): p. 483-492.

2.Zhang, L., et al. Room-temperature quaternary alkylammonium passivation toward morphology-controllable CsPbBr3 nanocrystals with excellent luminescence and stability for white LEDs. Chemical Engineering Journal, 2021. 417.

Phosphate removed by polyethylene imine/poly (methyl vinyl ether-alt-maleic anhydride) hydrogels

Jiangfeng Xu, Kirill Efimenko, Jan Genzer
Department of Chemical & Biomolecular Engineering, North Carolina State University

Background: Excessive phosphorus in the water can lead to eutrophication and the death of numerous aquatic animals. Phosphate is the primary form of phosphorus in water bodies. Chemical precipitation and enhanced biological phosphorus removal (EBPR) are currently used in wastewater treatment plants. Chemical precipitation demands precise stoichiometric additions, while EBPR necessitates careful control of pH and temperature. We are researching efficient phosphate sorbents that can be applied under ambient conditions.

Results: Hydrogels were synthesized by cross-linking polyethylene imine (PEI) with poly (methyl vinyl ether-alt-maleic anhydride) (PMVEMA). The sorption of P on the hydrogel was confirmed by infrared spectroscopy. The P removal efficiency was influenced by pH and PEI/PMVEMA ratio. We observed that the highest P sorption for PEI-rich hydrogel occurred at ~pH 5, whereas PMVEMA-rich hydrogel was at ~pH 4. The PEI-rich hydrogel exhibited a greater phosphate removal capacity (65 mg P per gram of sorbent) than the PMVEMA-rich hydrogel (12 mg P per gram of sorbent). We tested P desorption from hydrogels pre-absorbed with P to assess recycling potential. At pH 11, the pre-absorbed hydrogel released over 95% of the phosphates.

Conclusions: PEI/PMVEMA hydrogels have demonstrated exceptional phosphate capture abilities under acidic conditions while efficiently releasing phosphate under basic conditions. We could control the phosphate capture by adjusting the PEI/PMVEMA ratio and varying the pH.

References:

1. B. Wu, J. Wan, Y. Zhang, B. Pan and I. M. C. Lo, Environmental Science & Technology, 2020, 54, 50-66.

Millifluidic Flow Device for Accelerated Degradation Studies of Nonwovens

Lucille Verster [1, 2], Orlin D. Velev [1], Lokendra Pal [2]
1 . Dept. of Chemical and Biomolecular Engineering, NCSU; 2. Dept. of Forest Biomaterials, NCSU

Background: Synthetic polymer production has increased exponentially, significantly increasing plastic waste released into the environment[1]. Plastics can take many years to degrade while releasing persistent organic pollutants (POPs)[2]. In addition, degrading polymer waste poses a direct hazard to the environment and a direct and indirect danger to humans by releasing microplastic particles (MP). Remediating micro and nanosized plastic particles is one of today's most significant science challenges. This project aims to develop a novel millifluidic flow device (MFD) to characterize nonwoven degradation concerning environmental impact. To generate predictive models for this device, it is important to fully quantify, visualize, and characterize the degradation and photostability of fibers and nonwoven patches and analyze the results based on the major degradation mechanisms identified.

Results: Baseline experiments were conducted outside of the MFD. These experiments include characterizing microplastic fragment formation from nonwovens exposed to UV and elevated temperatures using different techniques. Changes in chemical composition were analyzed using Fourier Transform Infrared Spectroscopy – Attenuated Total Reflectance (FTIR-ATR), and physical strength was measured by doing tensile tests. In parallel with the baseline experiments, the MFD was developed and implemented by 3D printing. Currently, multiple MDF prototypes have been tested, and a robust operation device has been obtained. The MFD setup consists of a peristaltic pump to ensure DI water circulates the device, two chambers, where one is for nonwoven exposure, and the second chamber collects MP that has formed for further analysis, and a camera for continuous monitoring.

Conclusions: A reliable and suitable testing protocol for investigating the multiparametric mechanisms concerning UV degradation and MP release has been developed and verified. The initial tests provided insight into the experimental conditions and resulted in the early investigation of the effects of heat on degradation. The initial experiments also provided insight into the role of intensity of UV exposure. The latest prototype of reusable MFD shows robust usage and design.

References:

1. PlasticsEurope, 2021.Plastics - the Facts 2016: an Analysis of European Plastics Production, Demand and Waste Data Brussels, Belgium.
2. Deanin, R. D., “Additives in plastics”. *Environ. Health Perspect.*, **11**, 35-39 (1975).

CHTXS: An Automated Detector Program for Data Analysis of Chemotaxis Assays.

Daisy Aguilar [1], Andrew S. Clarck[1], Adriana San Miguel[1]
1. Dept. of Chemical and Biomolecular Engineering, North Carolina State University.

Background: Caenorhabditis elegans (*C. elegans*) is a transparent nematode (worm) organism with a well-characterized and compact neuron system [1] that enables analysis of behavior, molecular and chemosensory mechanisms, in fields of neurobiology, neurophysiology, toxicology, among others. *C*hemotaxis assays in *C. elegans* are widely used because they allow analysis of behavioral responses associated with neuronal function, relevant for analysis of neural circuits and even such as Alzheimer's disease (AD) due to the similar neuronal system between the nematode and the human.
Chemotaxis assay is a study of behavior based on the displacement of an organism like *C. elegans* driven by a chemosensory response to the exposure of certain chemical for a specific period of time (usually 60 minutes) . The chemotaxis assays are run on a petri-dish plate divided into two sides where a test chemical is placed at the end of one side of the plate and a null control at the other end with approximately 100-200 nematodes been placed at the center (initially). 24 total replicates are produced in a single chemotaxis assay: 6 replicates each for a positive control, for a negative control, a null control, and for the test chemical of our interest. These replicates help to ensure uniform responses to a chemical as well as to ensure the worms are in good health condition when exposed to these chemicals to validate any data obtained from the experiment[2].

Once the exposure time is completed, a manual counting process begins to obtain the chemotaxis index (CI) of each individual plate. CI measures an attractant or adversive response of the population. All replicates are counted manually using a microscope due to the length of the nematode (2mm maximum) which was a tedious and long process that potentially affected the overall CI on the plates because of the extended exposure time before being counted. We developed a new system that allows automated and quantitative analysis of chemotaxis in C. elegans, which uses two key technologies: a laser scanning system for capturing images of worms distributed in chemotaxis plates and an algorithm (CHTXS) that quantifies worm location within plates [2].

Results: The CHTXS detector program was created as an innovative and automated system focused on the analysis of chemotaxis experiments by efficiently reducing the counting time for all replicate plates as well as producing numerous diagrams, and plotted graphs regarding the CI values for each plate as well as for each control. The CHTXS detector program has the capacity to scan, detect, and analyze all replicates from a single chemotaxis assay at the same time by gathering the scanned images of all the controls (6 replicates in a single image), cropping the original images into each single plate to detect every nematode on each plate, and finally to create a summary table with the data obtained such as the CI value, final distance of every worm from the center, and visual diagrams of the final displacement of the worms across each plate as well as a summarized bar and boxplot graph containing all replicate results for each condition/control. The use of this program could potentially reduce the counting time frame and all the data analysis (including creation of tables, graphs, and diagrams) by up to 7 minutes (average) making the CHTXS detector program a novel automated system for chemotaxis assays.

Process Intensification Through Data-Rich Approach: Dynamic Exploration of Continuous Flow Quantum Dot Parameter Space

Hannah Dickerson [1], Fernando Delgado Licona [2], Milad Abolhasani [3]

1. Dept. Of Chemical & Biomolecular Engineering, North Carolina State University; 2. Escuela de Ingenieria y Ciencias, Technologico de Monterrey

Background: Recently, colloidal synthesis of II-VI and III-V Quantum Dot (QD) nanomaterial has been successfully achieved through the hot-injection and heat up synthesis batch process technique, resulting in near unity photoluminescence quantum yield and enhanced photostability[1]. To broaden QD integration in the renewable energy, display, and chemical industry, the search for more efficient QD nanomaterial and the corresponding sustainable manufacturing route has received increased attention in both academia and industry. This exploration through the QD synthesis space can be drastically accelerated by combining continuous flow chemistry and autonomous experimentation with reaction and data intensification. Specifically, applying process intensification in the form of microscale flow chemistry has demonstrated the ability to enhance heat and mass transfer through an increased surface to volume ratio, shortening startup and shutdown time, lowering reaction time, and decreasing precursor consumption, when compared to traditional batch chemistry. Moreover, continuous flow chemistry is capable of facile integration with data-rich experimental methodology, generating accurate *Big Experimental Data* for any precise physical and chemical condition[2]. However, most analyses performed in continuous flow chemistry discard the transient information obtained during experiment startup and shutdown, as well as between each experiment, consequently limiting data acquisition to only the steady state condition. Recuperating the discarded, transient information through data-rich experimental methodology can not only utilize data more effectively, but also significantly expedite the pace of research acceleration.

Results: In this work, we demonstrate the importance of analyzing transient phenomena for intensification of the experimental design space associated with nanoparticle synthesis through the systemic evaluation and optimization of the single stage continuous flow synthesis of an exemplary QD, cadmium selenide (CdSe). Additionally, we present reduced raw material consumption and lowered reaction timescales, relative to traditional steady state flow experimentation, thereby achieving considerable intensification of the development and discovery of colloidal functional material.

Conclusions: By embracing flow chemistry's compatibility with data-rich experimental methodology and extensively studying dynamic behavior, the pathway for accelerating experimentation is notably fortified, providing greater precision and efficacy for navigation of the complexity associated with QD discovery and development.

References:

1. Chen B, Li D, Wang F. (2020). InP Quantum Dots: Synthesis and Lighting Applications. *Wiley Online Library*. 16(32):2002454–2002454.
2. Delgado-Licona F, Milad Abolhasani. (2022). Research Acceleration in Self-Driving Labs: Technological Roadmap toward Accelerated Materials and Molecular Discovery. *Advanced Intelligent Systems*. 5(4).

Scalable Expression of LbCas12a Proteins in E. Coli

Jenna Kolbe [1], Zach Hetzler [1], Qingshan Wei [1]
1. Department of Chemical and Biomolecular Engineering, North Carolina State University

Background: CRISPR Cas proteins such as Cas12 and Cas9 proteins offer great opportunities for a wide range of sensing applications but at a high cost. When obtaining proteins for research commercially, it can cost the lab up to $1,000 for only 0.5 mg of LbCas12a [3]. The purpose of my project is to determine if we could produce needed proteins via a low-cost bacterial expression method utilizing the equipment and materials available in our lab. If successful, it would also allow for the purchase of plasmids that would produce other Cas proteins that are not commercially available, giving our research lab a wider range of CRISPR protein options. The overall process involves 1) plating the plasmid containing *LbCas12a* from the agar stab, 2) purifying it via Qiagen Miniprep, 3) transforming the plasmid into *E. Coli*, 4) cell growth and protein expression via fermentation, 5) cell lysis [1] and protein purification via affinity chromatography, and 6) protein characterization through BCA Assay, SDS-PAGE, and CRISPR diagnostics [2].

Results: We had roughly 2 mg of protein after purification from a one-liter fermentation. Characterization of the efficiency of the protein through CRISPR diagnostic assays as well as protein purity with SDS-PAGE was completed. The CRISPR diagnostic results combined with the SDS-PAGE results revealed that the purified fractions had little to no LbCas12a. Small-scale fermentations were conducted in 250 mL shake flasks under different conditions to determine the best conditions for cell growth and LbCas12a expression. The best conditions out of the ten tested were determined through SDS-PAGE. Two conditions expressed significantly more LbCas12a than the rest. They both had a final optical density of 600 nm of 6.0 and a final IPTG concentration of 0.75 mM. Only one parameter was different between the two, the optical density at 600 nm when the fermentation was induced with IPTG. One was 0.8 and the other was at 1.4.

Conclusions: The next steps are to use the two successful fermentation cultures to troubleshoot the purification process. Once characterization through SDS-PAGE and CRISPR diagnostics confirm that we have successfully expressed and purified LbCas12a, the process will be scaled-up to a two-liter shake flask with 400 mL of broth. Assuming the success of the larger-scale fermentation, this process will be translated to other Cas enzymes, such as Cas13.

References:

[1] Avhad DN, Rathod VK. 2014. Ultrasound stimulated production of a fibrinolytic enzyme. Ultrasonics Sonochemistry. 21(1):182-188. doi:https://doi.org/10.1016/j.ultsonch.2013.05.013.
[2] Chen JS, Ma E, Harrington LB, Da Costa M, Tian X, Palefsky JM, Doudna JA. 2018. CRISPR-Cas12a target binding unleashes indiscriminate single-stranded DNase activity. Science. 360(6387):436-439. doi:https://doi.org/10.1126/science.aat6245
[3] CRISPR-Cas12a (Cpf1) genome editing | IDT. Integrated DNA Technologies. https://www.idtdna.com/pages/products/crispr-genome-editing/alt-r-crispr-cpf1-genome-editing

Tunable Gradient Development Enables Exploration of Context-Dependent Cell Migration

James Kurdi [1], Joe Koelbl [1], Ravi Appalabhotla [1], Scott Baldwin [1], Jason Haugh [1]
1. Dept of Chemical Engineering, North Carolina State University

Background: Cell migration is essential to many functions that sustain multicellular organisms, such as immune response and tissue repair. Understanding the cues that drive cell migration could enable us to inhibit the errant migration that causes cancer metastasis or repair impaired wound healing in patients with chronic wounds like diabetic ulcers. An understudied type of cell motility of particular importance to wound healing is haptotaxis. Haptotaxis is the migration of a cell in response to an immobilized ligand. In the context of wound healing, this ligand is the extracellular matrix protein fibronectin. Fibroblasts, migratory cells involved in late stage wound healing, have been observed to denude, or remodel, extracellular matrix proteins as they migrate. This phenomenon results in a self-generated surface gradient that may influence fibroblasts' directed motility to wound sites. Since fibroblasts can modify external cues, their responses to said cues may be context-dependent. [1]

Results: Past studies have not explored cell migration across controlled gradient landscapes, so we have refined a highly tunable gradient generation technique to uncover context dependencies in migration. In this technique, called the meniscus method, a solution of fibronectin is applied to a microfluidic device consisting of polydimethylsiloxane (PDMS) bonded to a glass-bottom dish; the hydrophilicity of the dish confines the solution to a meniscus shape.

Conclusions: Using this method, we have generated gradients at controlled intensities. Preliminary results have shown context-dependent denuding in self-generated gradients, which we plan to explore further in controlled gradients produced by the meniscus method.

References:

[1] Bear, J. E., & Haugh, J. M. (2014). Directed migration of mesenchymal cells: Where signaling and the cytoskeleton meet. Current Opinion in Cell Biology, 30, 74–82. https://doi.org/10.1016/j.ceb.2014.06.005

Thermochemistry of Species in Gas-Phase Thermal Oxidation of C2 to C8 Perfluorinated Carboxylic Acids

H. Ram, C. C. Murphy, T. J. Mallo, P. R. Westmoreland*
Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, NC 27606

Background: Per- and poly-fluorinated alkyl substances (PFAS) were at one point widely used for many industries and consumer products. Among them, perfluorinated carboxylic acids and carboxylates (PFCAs) were produced using electrochemical fluorination processes beginning in 1947. Various formulations of Aqueous Film Forming Foams (AFFFs) consisted of various PFCAs and other PFAS and were developed starting from the 1960s and were used to fight fires. Sites that extensively used AFFFs to extinguish fires or train firefighters now have contaminated groundwater. PFAS, including PFCAs themselves, have been detected worldwide in wildlife and in human blood and plasma samples. Their potential for bioaccumulation is coupled with evidence for health effects such as increased cancer risk and immunotoxicity. The incineration of these "forever chemicals" is widely used as a method of remediation, but the chemical mechanisms of PFAS destruction remain understudied. The use of computational quantum chemistry and kinetic modeling techniques has had recent interest in this regard, and accurate gas-phase thermochemistry of the species involved is necessary. However, the use of expensive composite methods becomes computationally prohibitive with larger molecules that possess greater electron counts, which drives the use of cheaper alternatives such as density functional theory (DFT). We consider the full series of C_2 to C_8 PFCAs, and numerous species identified as potential participants in the mechanisms of pyrolysis and oxidation of those PFCAs.

Results: Thermochemical properties $C_p°(T)$, $H°(T)$, $S°(T)$, $G°(T)$, and bond dissociation energies are predicted for a wide range of species involved in the thermal destruction of C_2 to C_8 perfluorinated carboxylic acids (PFCAs) using computational quantum chemistry and ideal-gas statistical mechanics. 127 relevant species were identified from the development of mechanisms of the pyrolysis and oxidation of PFCAs C_2 to C_8 in length. Partition functions were obtained from the results of calculations at the G4 level for species up to C_4 in length and M06-2X-D3(0)/def2-QZVPP for species C_5 to C_8 in length. The 1D hindered-rotor approximation was used to correct for torsional modes in larger species. Thermochemistry was subsequently computed and fitted to 7-parameter NASA polynomials over a wide 10K-3000K temperature range, and the data are provided in standardized format. To gauge the effects of both method and basis set choice, 0 K formation enthalpies are calculated from various other density functionals (including B3LYP and ωB97XD), basis sets, and composite model chemistries (CBS-QB3). They are benchmarked against data from the Active Thermochemical Tables, high-level ANL0 calculations from the literature, and the G4 calculations carried out in this work. Effects of internal rotations and other anharmonicities are discussed, and relevant bond dissociation energies and reaction equilibria provide mechanistic insights.

Conclusions: Accurate thermochemistry is computed for 127 species involved in the pyrolysis and thermal oxidation of C_2 to C_8 perfluorinated carboxylic acids and benchmarked against literature and experimental data. Method comparisons are carried out, and insights from important bond dissociation energies and reaction equilibria are considered.

Risk Integration and Comparison Safety Study Between Generation II Light Water Reactors and Generation IV Non-Light Water Reactors

Elijah Rushing [1], Mihai A. Diaconeasa [2]
1. Dept. of Chemical and Biomolecular Engineering, North Carolina State University; 2. Dept. of Nuclear Engineering, North Carolina State University

Background: One of the concerns around nuclear energy is the safety associated with nuclear reactors due to radiation. It is believed that non-light water reactors (examples include reactors in which the coolants are helium, liquid metal, or molten salt; these are considered Gen IV reactors) can be as safe as or safer than previous generation light water reactors since Gen III+ reactors and Gen IV reactors rely on passive safety systems for all emergency conditions. The aim of this research is to examine and to compare the safety levels of non-light water reactors and light water reactors. To do this, the frequency and dose of event sequences of several reactors were graphed against the Frequency-Consequence Target graph described by the United States Nuclear Regulatory Commission. With the data that has been analyzed through probabilistic risk assessment and from current understanding of nuclear reactors, it is shown that that non-light water reactors can be as safe as or safer than light water reactors.

Results: The BWR and PWR from WASH-1400 had some frequencies that fell below 1E-10 per plant-year. One in ten billion years is around one event in the current assumed age of the universe. Therefore, anything that falls below this frequency is not what would be expected for this universe. This may be explained by PRA still being improved at the time that WASH-1400 was published. The data points from WASH-1400 used only the bottom-line probabilities and did not characterize, quantify, or include the uncertainties. As the Lewis committee concluded, a thorough uncertainty analysis, if an uncertainty analysis is not possible then a sensitivity study, should have been done to have a better understanding of the results [1]. Although, WASH-1400 did not include uncertainties with the bottom-line probabilities, the data can still be used; however, the data may need to be used with caution and awareness of the lack of uncertainty. As noted by all three reactors being below the frequency-consequence target, all three reactors meet the regulatory safety limits. Furthermore, due to being similar distances away from the frequency consequence target, the BWRs, PWRs, and HTGR-PBRs have similar safety levels. The BWR and the PWR are more closely related in terms of consequence as the data points associated with the BWR and the PWR are intertwined with one another. Out of the three reactors the HTGR-PBR had the lowest doses; however, the frequency was higher. The higher frequency can be explained by the lack of operational experience with HTGR-PBR.

Conclusions: In this study, the frequency and dose data were examined and compared for two light water reactors (BWR and PWR) and one non-light water reactor (HTGC-PBR). This study concluded that the non-light water reactor releases lower doses than the light water reactors. However, the non-light water reactor did have higher frequencies. This can be explained through the lack of operational experience that individuals have with the HTGC-PBR. However, all three reactors did meet the regulatory safety limits.

References:
1. “A Review of NRC Staff Uses of probabilistic Risk Assessment - NUREG-1489 - March 1994.pdf.”.

Understanding the Glass Transition Temperature of Felodipine/Cholic Acid Co-Amorphous Systems

Amelia L. Shea, Yung P. Koh, and Sindee L. Simon
Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, North Carolina, USA

Background: The glass transition temperature (T_g) and change in specific heat (ΔC_p) are investigated for co-amorphous mixtures of felodipine and cholic acid using differential scanning calorimetry (DSC). Co-amorphous mixtures are single-phase, binary systems that rely on molecular interactions and entropic effects between the two components to create a stable molecular glass [2]. In the area of pharmaceuticals, co-amorphous glasses are known to improve the drug bioavailability, solubility, and dissolution rate of the active pharmaceutical ingredient (API) compared to its crystalline structure [1]. The co-amorphous mixtures investigated in this research displayed a composition dependent T_g and ΔC_p. The composition dependence of co-amorphous mixtures are analyzed using theoretical models: the Fox, Gordon-Taylor, and Kwei equations. Additional dynamics related to the stability of these mixtures are briefly discussed.

Results: DSC was used to investigate the thermophysical properties of the pure felodipine and pure cholic acid and five mixtures on heating at 10 K/min after cooling at the same rate. All co-amorphous mixtures resulted in a single T_g and displayed no signs of melting indicating that there was no phase separation between felodipine and cholic acid. One of the five mixtures studied, 21% FEL, resulted in significant weight loss (>3%). The pure sample of felodipine showed T_g and ΔC_p values of 42.0 ± 0.7ºC and 0.22 ± 0.09 J/g/K, respectively. The pure sample of cholic acid showed T_g and ΔC_p values of 116.9 ± 0.7ºC and 0.62 ± 0.09 J/g/K, respectively. Five co-amorphous mixtures were studied: 21% FEL, 34.5% FEL, 44.8% FEL, 67.5% FEL, and 82.8% FEL. T_g and ΔC_p both decrease as the composition of FEL increases. Three theoretical T_g models were fit to the data: the Fox, Gordon-Taylor, and Kwei equations. The Fox and Kwei equations fit the data reasonably well resulting in an average error of 1.8 K and 2.3 K, respectively. The Gordon-Taylor resulted in an average error of 5.27 indicating that it does not fit the data well compared to the other two models.

Conclusions: The glass transition temperature regions of felodipine and cholic acid co-amorphous mixtures were investigated using differential scanning calorimetry. There is an observed composition dependence for both T_g and ΔC_p. The composition dependence of T_g is well described using the Fox and Kwei equations. Comparatively, the composition dependence of T_g using the Gordon-Taylor equation did not describe the data well. Future work will examine the dependence on cooling rate, and the stability of the co-amorphous materials against crystallization will be studied.

References:
1. Q. Shi, S. M. Moinuddin, T. Cai, "Advances in Coamorphous Drug Delivery Systems", *Acta Pharmaceutica Sinica B*, vol. 9, p. 19-35, 2019.
2. X. Zhao, S. Cheng, Y. P. Koh, B. D. Kelly, G. B. McKenna and S. L. Simon, "Prediction of the Synergistic Glass Transition Temperature of Coamorphous Molecular Glasses Using Activity Coefficient Models", *Molecular Pharmaceutics*, vol. 18, p. 3439–3451, 2021.

High-throughput single-cell sequencing of *B. fragilis* populations in the mouse gut

[1] Christine Stark, Freeman Lan [2], Ophelia Venturelli [2]
1. North Carolina State University, 2. University of Wisconsin - Madison

Background:
B. fragilis is a gram-negative gut commensal with eight capsular polysaccharides which could be expressed depending upon promoter expression. Capsular polysaccharides are essential as they contribute to the harmfulness of many gut pathogens as these capsular polysaccharides are able to hide cell-surface components which could trigger an immune response from the host [1]. This prompts the question regarding which capsular polysaccharides are selected for when the host undergoes various stressors. Through the use of high-throughput single-cell sequencing, promoter inversion and show was determined to be diverse in *B. fragilis* populations due to many capsular polysaccharide promoter states [2].

Results:
On day 29 the mice were inoculated with communities, thus increasing competition and selection within the mouse gut; consequently, variation decreased. By day 33 compositions with initially high capsular polysaccharide A proportions begin to experience less selection. This indicates a chance that capsular polysaccharide A does not play a significant role in the mouse gut. Furthermore, by day 33 those with low capsular polysaccharide H proportions begin to experience increased selection; thus, indicating the plausibility of capsular polysaccharide H playing a prevalent role in the mouse gut. Furthermore, capsular polysaccharides B and E seem to have a relationship as both proportions individually are low in the mouse gut as time progresses; however, when capsular polysaccharides B and E promoters are turned on in the same composition the proportion is exceptionally high. These results were confirmed when sequencing of the biological replicate occurred. On day 43, ATC is introduced into the mice's water supply. Furthermore, the introduction of ATC induced promoter scrambling resulting in increased variation.

Conclusions:
When looking at the data as a whole there is a chance that skewing occurred in the analysis process as those compositions containing ambiguities either in the form of “X” or “U” were removed. This could greatly affect the proportions and could account for some of the unexpected results. The next steps for this project include running the DoTA-seq workflow on the other experimental groups. Once compositions are obtained for all the experimental groups big picture conclusions can be made in regard to how the state/health of the mouse gut impacts capsular polysaccharide composition proportions.

References:
1. Cress, B. F., Englaender, J. A., He, W., Kasper, D., Linhardt, R. J., & Koffas, M. A. G. (2014, July). *Masquerading microbial pathogens: Capsular polysaccharides mimic host-tissue molecules*. FEMS microbiology reviews. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4120193/
2. Lan, F., Saba, J., Qian, Y., Ross, T., Landick, R., & Venturelli, O. S. (2022). *High-Throughput Single-Cell Sequencing of Multiple Invertible Promoters Reveals a Strong Determinant of Bacterial Population Heterogeneity*. https://doi.org/10.1101/2022.10.31.514637

High Throughput Mapping of Epigenetic Enzyme Activity

Katie Traynelis [1], Alison Waldman [1], Albert Keung [1], Balaji Rao [1, 2]
1. Dept. of Chemical and Biomolecular Engineering, North Carolina State University; 2. Golden LEAF Biomanufacturing Training and Education Center (BTEC), North Carolina State University

Background: Human DNA is organized into chromatin, which consists of DNA and associated proteins. Chromatin is a central regulator of gene expression, and therefore, its dysregulation and mutations in its regulatory components have been implicated in many disorders including cancer and neurodegeneration. A number of different reversible, chemical and biochemical groups can be added to DNA and to the histone proteins DNA associates with. These epigenetic modifications are a dynamic form of gene regulation and are thus of therapeutic interest. Here we focus on characterization of the amino acid sequence motifs that are acetylated by the epigenomic writer p300.

Results: A randomized 7mer yeast surface display library was constructed with a lysine at residue 4 and three randomized flanking amino acids on either side, giving a protein sequence diversity of $6.4x10^7$. A previously described yeast surface display platform was used to visualize protein expression, enzyme expression, and peptide acetylation [1]. The library was sorted using fluorescent activated cell sorting to isolate subpopulations of distinct acetylation levels, controlling for protein and enzyme expression. Multiple rounds of sorting were performed, and in the final round, the positive population was sorted into “medium” and “high” acetylation level populations. DNA of the subpopulations was sent for next generation sequencing, and Python scripts were used to identify amino acid sequence determinants of p300 acetylation. The workflow was performed with two separate anti-pan-acetyl-lysine antibodies, and enrichment of amino acid patterns as well as enrichment of specific sequences was observed. Amino acid patterns were observed when looking at the overall enrichment in each population, and there were differences between the populations collected with the two different antibodies. Specific sequence preferences emerged when certain residues were held constant in each population. Some of these sequence preferences were observed in the data sets generated from both antibodies.

Conclusions: The developed workflow is versatile and can be adapted to examine the specificity of other epigenetic writers. By examining p300, we were able to determine amino acid preferences as well as specific sequences that are acetylated to a greater extent by the writer. This expands overall understanding of the specificity of the writer and can be applied to a number of different protein engineering endeavors. A greater understanding of protein motifs that enhance acetylation by p300 advances overall scientific understanding of chromatin and its modifications.

References:

1. Waldman, Alison C., Rao, Balaji M., and Alber J. Keung (2021). Mapping the Residue Specificities of Epigenome Enzymes by Yeast Surface Display. *Cell Chemical Biol.*, 12: 1772-1779.

Graduate Student Resume Packet

Aniket Kapote

(919)-633-8288 ankapote@ncsu.edu linkedin.com/aniket-kapote

Education

North Carolina State University **Aug-2023 - May 2025**
Master of Science in Chemical Engineering *Raleigh, NC*

Visvesvaraya National Institute of Technology **Jul 2018 - May 2022**
Bachelor of Technology in Chemical Engineering | *GPA - 3.26/4* *Nagpur, India*

Technical Skills

Languages: Python, Java, C, C++, FORTRAN
Softwares: AmberTools, Gromacs, Matlab, Comsol, AspenPlus, Microsoft Office, Packmol, VMD
Technologies/Frameworks: Linux
Analytical Skills: HPLC, SDS-PAGE, Gel-Electrophoresis, UV-Spectrometry
Libraries: Seaborn, Pandas, Numpy

Relevant Coursework

- Chemical Process Modelling
- Reaction Engineering and Kinetics
- Emerging Nanomanufacturing Techniques
- Transport Phenomena
- Biochemical Engineering
- Cheminformatics
- Intro to Computational Software
- Advanced Separation Processes

Professional Experience

Reliance Industries Limited **Aug 2022 - April 2023**
Graduate Engineering Trainee *Navi Mumbai, India*

- Worked as a Graduate Engineering Trainee and Shift Engineer in a PX/PTA plant.
- Monitor and Supervise production processes during the shift to ensure smooth operation of the plant.
- Coordination of Start-Up and Shut-Down activities with the Inspection and Maintenance team to ensure all deadlines are met.
- Coordinating with Quality Assurance and Quality Control Lab to meet all product specifications.
- Ensuring all the OSHA-mandated safety standards are met in the plant.
- Prepared Hazard Identification and Task-based Risk Assessment files and gave training for the same.
- Preparing files for hydro testing of new as well as old pipelines
- Assessed the condition of equipment by doing calculations for parameters like Pressure Head, Heat Duty, etc.

QbD Purple Technologies Limited **Jun 2021 - August 2021**
Process Development Intern *Pune, India*

- Worked with a team of five to develop a process that separates lactoferrin from other whey proteins.
- Conducted experiments using cation exchange resin and a vertically packed bed column to test the separation of lactoferrin from other whey proteins.
- Further investigation included purification of the extracted component using microfiltration techniques.
- Minor project also included the separation of serum albumin from blood plasma.

Projects

Separation of Xylene Isomers using Carbon Nanotubes: A Molecular Dynamics Simulation Study
Guide - Dr. Piyush Wanjari **Apr 2021 - Mar 2022**

- Performed classical MD simulations using Carbon Nanotubes to study the separation of Xylene Isomers (p-Xylene, m-Xylene, o-Xylene)
- Designed scripts, codes, and input files for MD calculations with the use of Ambertools and Gromacs.
- Analysed and Compared the data obtained from the simulation run to obtain the best possible parameters for separating the isomers.

Studying CO2 Capture in Carbon Nanotubes with Ionic Liquids using Molecular Dynamics Simulation
Guide - Dr. Piyush Wanjari **Apr 2022 - Jun 2022**

- Performed Classical MD Simulations to study the ability of Ionic Liquids to entrap CO2 molecules in Carbon Nanotubes Cavity.
- Modelled, parameterized, and ran calculations using Ambertools and Gromacs for running classical MD Simulations.

Electrolyte Effect on CO2 Electroreduction

Dr. Nav Nidhi Rajput **Apr 2023 - Present**

- Performed AIMD and classical MD Simulation using MISPR and LAMMPS to calculate various properties for CO2 interaction with different classes of non-aqueous solvents.
- In this study, we investigate the use of nonaqueous solvents by using molecular simulations to examine the effect of the solvent's chemical class on properties relevant to the CO2 reduction reaction: CO2 solubility, electrochemical stability, and viscosity.

Leadership

Indian Institute of Chemical Engineers Students Chapter **Jun 2020 - Dec 2020**

Joint Secretary *Nagpur, India*

- Organized seminars where students connected with professionals from industries to gain an in-depth understanding of desired skills and current challenges of the industry.
- Conducted a national seminar on recent advancements in Chemical Engineering where researchers from various institutes presented their papers and posters.

Michael Bergman
Graduate Research Assistant – Prof. Carol Hall Group, North Carolina State University
mbergma2@ncsu.edu | (949) 330-0253 | Raleigh, NC

EDUCATION

B.S. Chemical Engineering: University of California, Los Angeles (*Summa Cum Laude, GPA 3.86)*
Sep 2012 – June 2016
PhD., Chemical Engineering: North Carolina State University, Carol Hall Group
Aug 2020 – Present

WORK AND RESEARCH EXPERIENCE

Graduate Researcher – *Carol Hall Group, NC State University, Raleigh, NC*
Jan 2021 – Present

- Investigating the thermodynamic driving forces of peptide adsorption to polymers using molecular dynamics simulations
- Developing a Monte Carlo algorithm that designs peptides with high affinity for plastics, where the designed peptides will be facilitate detection, capture, and degradation of microplastic pollution
- Collaborating with researchers at Cornell university to apply quantum annealing, reinforcement learning, and graph neural networks into the peptide design process
- Determining the mechanism of *trans* DNA cleavage by the activated Cas12a enzyme using molecular dynamics and docking methods

Volunteer Researcher – *Ruth Nussinov Group, NIH Cancer Innovation Laboratory, Frederick, MD*
June 2023 – Present

- Exploring the structural features that give rise to specific cyclin:cyclin-dependent kinases complexes necessary for cell-cycle progression via protein-protein docking
- Analyzing the stability and activity of atypical complexes to determine if they merit consideration in basic cell biology and development of effective treatments for cancer and neurodegenerative diseases

Drug and Medical Device Engineer: *Abbott Laboratories, Sylmar, CA*
Oct 2019 – Aug 2020

- Led development of drying process for a thermally sensitive steroid used to reduce inflammation during surgical implantation of pacemakers

Process Engineer II: *Applied Medical, Rancho Santa Margarita, CA*
Jan 2017 – Aug 2018

- Reduced cost of cauterizing device by 15% by co-leading a project to validate a metal injection molding process to manufacture metal components of cauterizing surface
- Improved thermal and pressure uniformity of cauterizing device by validating a thermal spraying procedure that precisely controlled key geometric properties of the cauterizing surface
- Initiated investigation of polymer coating to reduce tissue build-up on cauterizing surface during surgery
- Mentored an intern in the design of inspection equipment and qualification of manufacturing equipment

Research Associate - Intern: *Genefluidics, Duarte, CA*
June 2015 – Aug 2018

- Increased signal strength of an immunoassay biosensor by 10% by optimizing assay parameters via design of experiments

- Investigated the efficacy of cryogenic storage in improving shelf life of biosensors

Research Assistant: *Julio Vergara Group, University of California, Los Angeles*
May 2014 – June 2015

- Increased durability and decreased assembly complexity of a form-fitting, programmable thermoregulation device by testing and introducing new polymer materials and manufacturing methods
- Improved steady-state response time and stability of the device's temperature regulation by increasing its heat transfer properties

TEACHING EXPERIENCE

- **Teaching Assistant:** Undergraduate thermodynamics 2 (Spring 2023), graduate thermodynamics 1 (**Fall 2022**), graduate transport phenomena (**Spring 2022**), undergraduate thermodynamics 1 (**Fall 2021**)
- **Tutor:** Academic Learning Labs (**09/2018 – 8/2019**); Tutor Club (**09/2016 – 12/2016**)

SELECTED OUTREACH ACTIVITIES

- **Teacher/Coordinator:** The Science House, NC State University – created microplastic aggregation simulation and associated lecture materials to educate middle and high school students about how simulations can investigate the behavior of microplastics
- **Teacher**: NC School for the Deaf – Created lecture materials to educate students about antibodies
- **Graduate Student Organizer:** 2022 NC State BioLunch Seminar Series
- **Graduate Student Organizer**: 2022 NC State Future Leaders in Chemical Engineering Symposium
- **Mentor**: Peer Mentor Program in NC State University Chemical Engineering Department (2021, 2023)

PUBLICATIONS

- **Bergman, M**. T.; Xiao, X.; Hall, C. K. In Silico Design and Analysis of Plastic-Binding Peptides. J. Phys. Chem. B 2023. https://doi.org/10.1021/acs.jpcb.3c04319.
- Bang, R. S.; **Bergman, M**.; Li, T.; Mukherjee, F.; Alshehri, A. S.; Abbott, N. L.; Crook, N. C.; Velev, O. D.; Hall, C. K.; You, F. An Integrated Chemical Engineering Approach to Understanding Microplastics. AIChE J. 2023, 69 (4), e18020. https://doi.org/10.1002/aic.18020.
- Harris, F. R.; Sikes, M. L.; **Bergman, M**.; Goller, C. C.; Hasley, A. O.; Sjogren, C. A.; Ramirez, M. V.; Gordy, C. L. Hands-on Immunology: Engaging Learners of All Ages through Tactile Teaching Tools. Front. Microbiol. 2022, 13.
- *In preparation*: Combining Biophysics, Quantum Computing, and Reinforcement Learning to Design Plastic Binding Peptides
- *In preparation:* Exploring the Structural Features that Give Rise to the Affinity and Specificity of CDK-Cyclin Complexes For Progression Through the Cell Cycle

SKILLS AND INTERESTS

Computational: Python, Fortran, Matlab, Amber, Gromacs, Plumed, VMD, Monte Carlo methods, Docking, Molecular dynamics simulations, Mathematical Modeling, Neural Networks
Engineering: Process Development, Statistical Analysis, Design of Experiments
Hobbies: Guitar, Piano, Crossword Puzzles, Ultimate Frisbee, Hiking, Board Games, Reading

Ryan G. Bing

Address: 2021 Fieldhouse Ave.
Raleigh, NC 27603

Phone: 515-868-2537
Email: ryangbing96@gmail.com

Education

- **North Carolina State University, Raleigh, NC (Aug. 2018 – May 2024, expected)**
  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: Jan. 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*.
- **Pfizer, MSAT Graduate Intern, Sanford, NC**: **May – Aug. 2023**
  Created computation fluid dynamics models of several processes targeted towards improving process efficiency and understanding.
- **Undergraduate Research, Dr. John Morgan Lab, Purdue: Aug. 2016 – May 2018**
  Characterized volatile organic compounds' (VOCs) transport and emission through petunia petal cuticle layer to understand physical and biological mechanisms controlling plant VOC synthesis and emission.
- **Undergraduate Research, Dr. Boudouris Lab Group, Purdue: Aug. – Dec. 2017**
  Determined the effect of humidity on the conductivity of polymers (PTMA and PTNB).
- **Rolls Royce, Materials Technology Center Intern, Indianapolis: May – Aug. 2017**
  Analyzed coatings for jet engine components for elimination of toxic materials and optimization in marine environments, validated alternative fuels for use in jet engines.
- **Dow AgroSciences**, **Competitive Intelligence Intern, Indianapolis: May – Aug. 2016**
  Compiled information on key competitors and developed a user interface in Tableau to analyze the data; final product was released globally within Dow AgroSciences.
- **Dow AgroSciences, Automation Group Intern, Indianapolis: May – Aug. 2015**
  Developed processes to miniaturize and refine several genotyping laboratory processes to reduce costs using nano and microliter scale liquid-handling machines.
- **Rolls Royce, Quality Control Intern, Indianapolis: Jun. – Aug. 2014**
  Contracted through Belcan Corporation, analyzed jet engine parts for metallurgical defects.

Affiliations

- Review Editor for Frontiers in Microbiology, Extreme Microbiology: Apr. 2023-present
- American Chemical Society: Aug. 2014 – present
- American Institute of Chemical Engineers: Jan. 2015 – present

Volunteer and Community Service

- Mentor for four undergraduates in biotechnology research, Jan. 2020-present
- Assist with Graduate Student Recruitment for CBE Dept. at NCSU, Mar. 2019 - present
- Organized & presented biotechnology seminar for Grade 9-12, Ankeny High School, IA, 26 Nov. 2019

Awards

- US NIH Biotechnology Traineeship (T32 GM008776-20, GM133366-01) (2019-2021)
- North Carolina State University Graduate Fellowship (2018-2019)

Publications

1. **Bing RG,** Willard DJ, Crosby JR, Adams MWW, Kelly RM. *Wither the Genus Caldicellulosiruptor and the Order Thermoanaerobacterales: Phylogeny, Taxonomy, Ecology, and Phenotype*. Frontiers Microbiol (2023)
2. **Bing RG,** Willard DJ, Manesh MJH, Laemthong T, Crosby JR, Adams MWW, Kelly RM. *Complete Genome Sequences for Two Thermophilic Indigenous Bacteria Isolated from Wheat Straw: Thermoclostridium stercorarium subsp. RKWS1 and Thermoanaerobacter sp. RKWS2.* Microbiol Resour Announc (2023).
3. **Bing RG**, Willard DJ, Manesh MJH, Laemthong T, Crosby JR, Adams MWW, Kelly RM. *Complete Genome Sequences of Caldicellulosiruptor acetigenus DSM 7040, Caldicellulosiruptor morganii DSM 8990 (RT8.B8), and Caldicellulosiruptor naganoensis DSM 8991 (NA10).* Microbiol Resour Announc (2023).
4. **Bing RG**, Carey MJ, Laemthong T, Willard DJ, Crosby JR, Sulis DB, Wang JP, Adams MWW, Kelly RM. *Fermentative conversion of unpretreated plant biomass: A thermophilic threshold for indigenous microbial growth*. Bioresour Technol (2022).
5. **Bing RG**, Straub CT, Sullis DB, Wang JP, Adams MWW, Kelly RM. *Plant Biomass Fermentation by the Extreme Thermophile Caldicellulosiruptor bescii for Co-Production of Green Hydrogen and Acetone: Technoeconomic Analysis.* Bioresour Technol (2022).
6. **Bing RG,** Sulis DB, Wang JP, Adams MWW, Kelly RM. *Thermophilic microbial deconstruction and conversion of natural and transgenic lignocellulose*, Environ Microbiol Rep (2021).
7. Tanwee, TNN, Lipscomb GL, Vailionis JL, Zhang K, **Bing RG**, O'Quinn HC, Poole FL, Zhang Y, Kelly RM, Adams MWW. *Metabolic Engineering of Caldicellulosiruptor bescii for 2,3-butanediol Production from Lignocellulosic Substrates and Metabolic Strategies for Improving Yields and Titers.* (Under Review, 2023).
8. Sulis DB, Jiang X, Yang C, Marques BM, Matthews ML, Miller Z, Lan K, Cofre-Vega C, Liu B, Sun R, Sederoff H, **Bing RG**, Sun X, Williams CM, Jameel H, Phillips R, Chang HM, Peszlen I, Huang YY, Li W, Kelly RM, Sederoff RR, Chiang VL, Barrangou R, Wang JP. *Multiplex CRISPR editing of wood for sustainable fiber production.* Science (2023).
9. Vailionis JL, Zhao W, Zhang K, Rodionov DA, Lipscomb GL, Tanwee TNN, O'Quinn HC, **Bing RG**, Kelly RM, Adams MWW, Zhang Y. *Optimizing Strategies for Bio-Based Ethanol Production Using Genome-Scale Metabolic Modeling of the Hyperthermophilic Archaeon, Pyrococcus furiosus*. Appl Environ Microbiol, (2023).
10. Laemthong TL, **Bing RG**, Crosby JR, Manesh MJH, Adams MWW, Kelly RM. *Role of cell-substrate association during plant biomass solubilization by the extreme thermophile Caldicellulosiruptor bescii.* Extremeophiles (2023).
11. Crosby JR, Laemthong T, **Bing RG**, Zhang K, Tanwee TNN, Lipscomb GL, Rodionov DA, Zhang Y, Adams MWW, Kelly RM. *Biochemical and Regulatory Analysis of Xylanolytic Regulons in Caldicellulosiruptor bescii Reveal Genus-Wide Features of Hemicellulose Utilization.* Appl Environ Microbiol (2022)
12. Laemthong T, **Bing RG,** Crosby JR, Adams MWW, Kelly RM. *Engineering Caldicellulosiruptor bescii with Surface Layer Homology Domain-Linked Glycoside Hydrolases Improves Plant Biomass Solubilization.* Appl Environ Microbiol (2022).
13. Laemthong T, Lewis AM, Crosby JR, **Bing RG,** Schneider WH, Willard DJ, Counts JA, Kelly RM. *Enzymes from extremely thermophilic bacteria and archaea: Current status and future prospects.* Chapter 1 in Extremozymes and their Industrial Applications, Academic Press (2022).
14. Rodionov DA, Rodionova IA, Rodionov VA, Arzamasov AA, Zhang K, Rubinstein GM, Tanwee TNN, **Bing RG,** Crosby JR, Nookaew I, Basen M, Brown SD, Wilson CM, Klingeman DM, Poole FL, Zhang Y, Kelly RM, Adams MWW. *Transcriptional regulation of plant biomass degradation and carbohydrate utilization genes in the extreme thermophile Caldicellulosiruptor bescii,* mSystems (2021).
15. Zhang K, Zhao W, Rodionov DA, Rubinstein GM, Nguyen DMN, Tanwee TNN, Crosby JR, **Bing RG**, Kelly RM, Adams MWW, Zhang Y. *Genome-scale metabolic model of Caldicellulosiruptor bescii reveals optimal metabolic engineering strategies for bio-based chemical production,* mSystems (2021).
16. Straub CT, **Bing RG,** Otten JK, Keller LM, Zeldes BM, Adams MWW, Kelly RM. *Metabolically engineered Caldicellulosiruptor bescii as a platform for producing acetone and hydrogen from lignocellulose*, Biotechnol Bioeng (2020).
17. Straub CT, **Bing RG,** Wang JP, Chiang VL, Adams MWW, Kelly RM. *Use of the lignocellulose-degrading bacterium Caldicellulosiruptor bescii to assess recalcitrance and conversion of wild-type and transgenic poplar.* Biotechnol Biofuels 13, 43 (2020).
18. Lee LL, Crosby JR, Rubinstein GM, Laemthong T, **Bing RG,** Straub CT, Adams MWW, Kelly RM. *The biology and biotechnology of the genus Caldicellulosiruptor: recent developments in 'Caldi World'.* Extremophiles 24, 1–15 (2020).

References available upon request.

LEO G. BRODY · lbrody@ncsu.edu · (919) 741-8913 · Raleigh, North Carolina, 27603

EDUCATION

North Carolina State University · *Raleigh, N.C.*
Ph.D. · Chemical and Biomolecular Engineering **2020 - Present**
M.S. · Chemical and Biomolecular Engineering **2019 - 2021**
American University · *Washington, D.C.*
B.S. · Environmental Science · Mathematics minor **2012-2016**

SKILLS AND PROFICIENCIES

- Technical: Design and automation of bench-and sub-pilot-scale heterogeneous catalytic reactors for gas, liquid, and solid feeds including packed-bed and fixed fluidized bed reactors; catalyst characterization; Rietveld refinement; solid-state synthesis; chemical process modeling; gas-solid kinetic modeling; and scientific communication.
- Software: GSAS-II, HighScore, FullProf Suite, ASPEN Plus, CasaXPS, LabVIEW, Origin, Microsoft Office.
- Foreign languages: French (full professional proficiency), and German (elementary proficiency).

RESEARCH EXPERIENCE

Graduate Research Assistant **2019 – Present**
North Carolina State University · Chemical and Biomolecular Engineering · *Raleigh, N.C.*
Thesis advisor: Prof. Fanxing Li

(i) Thesis project: Phase Transition CO_2/O_2 Sorbent Enhanced Chemical Looping Gasification of Biomass for Renewable Syngas Production
- Synthesized and characterized unique classes of mixed metal oxide catalytic sorbents using DSC-TGA, H_2/CO_2-TPR, FTIR, *ex-situ* and *in-situ* XRD, XPS, BET/BJH, TOF SIMS, TEM, and SEM/EDS.
- Designed, constructed, and automated bench-scale experiments using LABVIEW and other software for cyclic liquid, solid, and gas injections with temperature swings.
- Performed detailed synchrotron in-situ XRD data analysis using Rietveld refinement to determine the underlying solid-state chemistry that enables successful sorbent performance.

(ii) Modular gas to liquids via chemical looping-based oxidative dehydrogenation of ethane
- Designed, constructed, and operated small and large bench-scale as well as pilot-scale packed bed reactors for the use of redox catalysis experiments.
- Constructed and automated gas panels programmed via LabVIEW for cyclical gas injections and performed materials characterization to investigate catalyst deactivation over long-term cycling.
- Simulated chemical processes and conducted sensitivity/techno-economic analysis using ASPEN Plus and Excel.

Visiting Graduate Researcher
Technische Universität Berlin · Institut für Chemie · *Berlin, Germany* **2022-2023**
- Conducted research with the group of Prof. Dr. Reinhard Schomäcker in the Department of Reaction Engineering at TU Berlin on phase transition sorbent characterization using XAFS and synchrotron in-Situ XRD.
- Performed packed bed experiments to uncover the mechanism of a complex, multi-phase catalyst for oxidative coupling of methane.

PUBLICATIONS

1. **Brody, L.,** Rukh, M., Cai, R., Bosari, A.S., Schomäcker, R, and Li, F. "Sorption-enhanced steam reforming of toluene using multifunctional perovskite phase transition sorbents in a chemical looping scheme". *Journal of Physics: Energy,* **2023**, 5, 035004.
2. Cai, R., **Brody, L.,** Tian, Y., Neal, L., Bose, A., and Li, F. "Numerical Modeling of Chemical Looping Oxidative Dehydrogenation of Ethane in Parallel Packed Beds". *Chemical Engineering Journal*, **2023**, 469, 143930.
3. Ruan, C. Akutsu, R., Yang, K. Zayan, N., Dou, J., Liu, J., Bose, A., **Brody, L.,** Lamb, H., and Li, F. "Hydrogenation of bio-oil oxygenates at ambient conditions via a two-step redox cycle". *Cell Reports Physical Science.*
4. **Brody, L.,** Neal, L., Liu, J., and Li, F. "Autothermal Chemical Looping Oxidative Dehydrogenation of Ethane: Redox Catalyst Performance, Longevity, and Process Analysis". *Energy and Fuels*, **2022**, 36, 17, 9736-9744.

5. **Brody, L.,** Cai, R.,* Thornton, A., Liu, J., Yu, H., and Li, F. "Perovskite-based Phase Transition Sorbents for Sorption Enhanced Oxidative Steam Reforming of Glycerol". *ACS Sustainable Chemistry and Engineering,* **2022**, 10, 19, 6434-6445. *Co-first author.
6. **Brody, L.,** Neal, L.,* Haribal, V., and Li, F. "Ethane to liquids via a chemical looping approach – Redox catalyst demonstration and process analysis". *Chemical Engineering Journal*, **2021**, 417, 128886. *Co-first author.

PATENTS

Li, F., **Brody, L.,** Cai, R., Rukh, M., and Yang, K. Multi-functional catalytic sorbents for hydrogen and hydrogen-enriched syngas production from carbon-containing feedstock.

POSTERS AND PRESENTATIONS

1. **Brody, L.,** Cai, R., Rukh, M., Müller, J., Bekheet, M., Gao, W., Schomäcker, R, and Li, F. Perovskite-based Phase Transition Sorbents for CO_2 Sorption-Enhanced Oxidative Steam Reforming. *The 15th European Congress on Catalysis*, Prague, Czech Republic. 27 August **2023**. (Oral)
2. **Brody, L.,** Cai, R., Rukh, M., Thornton, A., and Li, F. Sustainable Syngas Production via Sorption Enhanced Biomass Gasification. *KIETS Climate Leaders Symposium*, Kenan Institute, NCSU, Raleigh, N.C., 9 October **2022**. (Poster).
3. **Brody, L.,** Gao, Y., Wang, X., Liu, J., Neal, L., and Li, F. Molten salt promoted perovskite redox catalysts for anaerobic oxidative dehydrogenation of light alkanes. *The 27th North American Catalysis Society Meeting*, New York City, NY, 23 May **2022**. (Oral)
4. **Brody, L**., Cai, R., Dou, J., Thornton, A., and Li, F. Sustainable Syngas Production via Sorption-enhanced Steam Reforming of Bioglycerol. *Schoenborn Graduate Research Symposium*, CBE Department, NCSU, Raleigh, N.C., 28 September **2021**. (Poster)
5. **Brody, L**. The Role of Chemical Looping Technology in Chemical Engineering Pedagogy. *ASEE Annual Conference.* Virtual presentation, **2021**. (Oral).
6. **Brody, L**. Ethane to Liquids via a Chemical Looping Approach – Redox Catalyst Demonstration and Process Analysis. *Carolina Science Symposium*. Virtual presentation, 13 November **2020**. (Oral)
7. **Brody, L**., Dizio, B., and Dumiak, J. Topological Data Quality Assessment for Sonar Targets and Homological Features for Sonar Target Classification. *February Fourier Talks*, University of Maryland, 19 February **2015**. (Poster)

TEACHING EXPERIENCE

Graduate Teaching Assistant
CHE 316 · Thermodynamics of Chemical and Phase Equilibria· *CBE Department, NCSU*, **2022**
CHE 205 · Chemical Process Principles · *CBE Department, NCSU*, **2021**
CHE 596-606/607 · Core Chemical Engineering Concepts I/II · *CBE Department, NCSU*, **2020-2021**

HONORS AND AWARDS

- KIETS Climate Leaders Scholar · *Kenan Institute, NCSU,* **2023**
- Linde Exceptional Teaching Assistant Award (finalist) · *CBE Department, NCSU*, **2022**
- Best graduate student design entry · *ASEE DEED Design Vision Competition,* **2021**
- Best student oral presentation, session four · *Carolina Science Symposium,* **2020**
- College of Engineering Graduate Merit Award · *NCSU,* **2020**

SERVICE AND VOLUNTEERING

Co-Founder and Director **2014-2016**
D.C. Students for STEM Education · *Washington, D.C.*

- Co-founded a 501(c)-3 with the aid of United Charitable during my sophomore year of college.
- Directed an education non-profit to provide free STEM education packages to public schools, after-school centers, and housing projects in Washington, D.C.
- Provided one year's worth of monthly STEM lessons to the Jubilee Housing project and collaborated with the Maryland chapter of Bricks 4 Kidz.
- Organized local fundraisers as well as oversaw a volunteer staff of 10 undergraduates.

Nate Brown

1250 Silver Beach Way
Raleigh NC 27606
www.linkedin.com/in/nate-brown-15917
(336) 423-2865
nabrown4@ncsu.edu

North Carolina State University, Raleigh, North Carolina *May 2024*
Ph.D. Material Science and Engineering
GPA: 3.58
B.S. Chemical Engineering *May 2019*
GPA: 3.75

Coursework:
Crystallography Diffraction, Data Informatics, Materials Informatics, Polymer Tech. and Eng., Mech. Behavior of Mat., Statistics, Uncertainty Quant., Biomaterials Eng., Interfacial Polymers, Thermodynamics, Polymer Rheology

Publications
- H. Kim, N. Brown, S. Zauscher, Y. Yingling. 2020. "Effect of Octadecylamine Surfactant on DNA Interactions with Graphene Surfaces" *Langmuir*, 36(4), 931-938

Work Experience
- **Graduate Research Assistant in Grenzer Interfacial Research Laboratory (GIRL)**
  Raleigh, NC *May 2020 - Current*
  - Developed hydrogel reactors for tailored interfacial chemistry, enabling drag-drop polymerizations under mild conditions
    - Developed in-depth understanding of ligand-metal charge transfer (LMCT) mechanism from literature analysis driving segment modeling study of significant biopolymer groups via UV-Vis analysis revealing the correlation between biopolymer functional group presence and LMCT
    - Utilized previous findings and further literature search to develop a biopolymer system capable of metal reduction for surface-initiated metal-ligand polymerizations
    - Established standard operating procedure to learn, rapidly synthesize, and analyze 15+ surface-initiated Atom Transfer Radical Polymerizations, providing consistent quality of results correlating the presence of functional groups to self-chelating behavior and promoting polymerization in ligand absence
    - Constructed polymer-gel-based systems for specialized monomers and improved hydrogel swelling with FTIR analysis to confirm biopolymer modification
    - Conducted FTIR and ellipsometry analysis on polymer brushes synthesized via gel system to confirm polymer brush species and formation
  - Trained and recommended procedures for graduate and undergraduate students resulting in significant increase in polymer yields pertaining to ATRP reactions
  - Trained in FTIR (ATR and Transmission), Ellipsometry, CA Goniometry, UV-Vis, SI-ATRP, Spin-Coating, and soxhlet/continuous extraction for sample analysis and understanding of ligation chemistry
- **Lab Safety Officer in Genzer IRL**
  - Completed safety training and documentation for 25 graduate and undergraduate students while maintaining an EHS-compliant laboratory
  - Coordinated and directed bi-weekly safety meetings with a graduate team of 4 to systematically organize lab spaces and replenish regularly used lab materials.
- **Undergraduate Research Assistant for Optimization of InGaN Green Emission LEDs**
  Raleigh, NC (40 hours/week) *May-August 2019*
  - Developed and applied an understanding of nano-defects and superlattices to band-gap materials while learning SOP for metal-organic chemical vapor deposition technique for the synthesis and analysis of InGaN LEDs with specialized focus on green wavelength emissions
  - Learned and applied photo-luminescence and X-ray diffraction analytical techniques for determining the emission wavelength and material thickness of grown diodes
- **Undergraduate Researcher in Nano-Science Engineering and Research Group**
  Raleigh, NC (20 hours/week) *March 2018 - 2019*
  - Improved thermoelectric figure of merit ZT by 68% through focused minimization of contamination and increased emphasis on accuracy for metal-alloyed materials
  - Trained in LSR, XRD, LFA, Hot-Press metal Sintering, and Melt-Quenching techniques, boosting result acquisition within one month period

- **Undergraduate Researcher in Yingling Soft Materials Simulations and Informatics Group**
  Raleigh, NC (20 hours/week) *March 2017 – March 2018*
  - Displayed proficiency in independent data analysis through the utilization of Microsoft Excel, Visual Molecular Dynamics, and Amber 2016 for the study of biopolymer denaturation on graphene 2-dimensional sheets, resulting in co-author publication
  - Showcased results orally and visually at Graduate and Undergraduate level symposiums and awarded certificates of outstanding accomplishment and contributions

Awards and Fellowships

- **SEAS Trainee Fellowship** *March 2020 – December 2021*
  - Developed and applied background in machine learning and data informatics for streamlined research analysis
- **Mentored Teaching Fellowship** *January 2020 – May 2020*
  - Established and taught hands-on lab curriculum drawing from relevant coursework for improved understanding and application of outlined theory and lab techniques

Engineering Experience

- Hobbyist AutoCAD engineer with applied experience in prototype conceptualization, design, and fabrication
  - Learned Fusion360 to design (30 hours) an entirely 3D printed multistep puzzle box including a blind labyrinth, 4-digit lock, and Geneva wheel locking mechanism
  - Finetuned AutoCAD design and tolerances in conjunction with optimized 3D printing conditions to obtain a sub-millimeter level of precision in printed mechanical designs and minimal post-processing

Community Involvement and Volunteer Experience

- **Material Science Mentorship Program** *September 2022-Current*
  - Serving as Mentor for 2nd year Master's student, providing insight into Ph.D. as well as project-related advice on organization, experimental design, and establishing focused objectives
- **Homework Club of Hope Church** *September 2020-Current*
  - Optimized tutors-student pairings based on tutor expertise and student needs, resulting in academic improvement and growth of the Homework Club ministry
  - Collected and directed parents to accessible resources for students with additional tutoring requirements, including counseling, extracurricular sports, and special needs
- **Tabletop Game Lead**
  - Developed new skill sets (< 6 months) combining AutoCAD, foam modeling, organic architectural designs, and standard operating procedures for the production of complex 3D modular sets, enabling a high level of quality and detail while minimizing production cost and construction time
  - Tabletop game lead consisting of 5+ players while creating an inclusive and welcoming environment that enables independent creativity and complex storytelling

Nidhi Diwakar

919-601-5142
nmdiwaka@ncsu.edu

Summary

Fifth 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 — Aug 2019 – Present
Ph.D., Chemical Engineering
(GPA 3.634)

North Carolina State University (NCSU), Raleigh, NC — Aug 2019 – Dec 2021
MS, Chemical Engineering
(GPA 3.634)

Worcester Polytechnic Institute (WPI), Worcester, MA — Aug 2012 – May 2016
BS, Robotics Engineering
(GPA 3.6, High Distinction)

Research Experience

PhD Researcher, NCSU — Jan 2019 – Present

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

- Investigating electrohydrodynamic effects of temporally nonuniform AC field-driven active particles
- Characterizing and modeling behavior of previously unreported AC field effects
- Exploring collective behavior of superdiffusive salt paste in chemical gradients
- Working towards biomedical application of superdiffusive paste for dermal disinfection
- Conducting cytotoxicity testing via contact and diffusion assays

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

Presentation, "Active Particle Propulsion Due to Temporally Asymmetric AC fields", *97th ACS Colloid and Surface Science Symposium* — 2023

Poster, "Active particle propulsion due to temporally asymmetric AC fields", *Gordon Research Conference on Colloidal, Macromolecular and Polyelectrolyte Solutions* — 2022

Poster, "New Principles of Active Particle Propulsion Driven by Electrical and Chemical Gradients", *14th International Symposium on Electrokinetics (ELKIN)* — 2022

Coauthor, "AC Electrohydrodynamic Propulsion and Rotation of Active Particles of Engineered Shape and Asymmetry", *Curr. Opin. Colloid Interface Sc.* — 2022

Poster, "New Principles of Active Particle Propulsion Driven by Electrical and Chemical Gradients", *Schoenborn Research Symposium*, NCSU — 2021

Presenter, " Superdiffusive paste from active particles driven by collective phenomena of ionic salt dissolution", *95th ACS Colloid and Surface Science Symposium* — 2021

Presenter, "Asymmetric AC Field Powered Propulsion of Active Particles", *Triangle Soft Matter Workshop* — 2021

Presenter, "AC Field Powered Propulsion and Light Controlled Steering of Engineered Active Particles", *Triangle Soft Matter Workshop* — 2020

Coauthor, "Sequence-encoded colloidal origami and microbot assemblies from patchy magnetic cubes", *Sci. Adv.* 2017; 3, e1701108. 2017

Teaching and Leadership Experience

Student Organizer, 97th ACS Colloid and Surface Science Symposium	Mar – Jun 2023
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 – May 2023

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 following ITAR regulations
- 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

Honors and Awards

NCSU Envisioning Research Award: 2nd place in video	Aug 2023
Graduate Student Association Travel Award	Nov 2022

Skills and Proficiencies

Optical Microscopy, Dynamic Light Scattering, Blender, Solidworks, MATLAB, Origin Lab
Experience in cell culture, contact and diffusion assays, top agar method
Highly proficient in physical vapor deposition
Kannada, French, German

MATTHEW A. DORSEY

LinkedIn: https://www.linkedin.com/in/matthewadorsey | **GitHub:** https://github.com/sunprancekid

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

+1 (314) 745-3514
mdorsey113@gmail.com

OBJECTIVE

My objective is to develop my career as a Scientific Software Developer. I am excited about developments being made in the pharmaceutical, biotechnology, and life sciences fields. I believe that the most effective, data-driven solutions come by integrating an understand of mathematical physics, physical chemistry and molecular biology with computational models and computing systems.

SUMMARY OF QUALIFICATIONS

- Experienced developing scientific software applications for High Performance Computing (HPC) clusters
- Background in topics related to physics, chemistry, molecular biology, and mathematics
- Completing a Doctor of Philosophy in Chemical Engineering

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 with bash scripts** that submit large numbers of computing jobs with varying initial conditions to HPC clusters and 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
- Summarized results of molecular simulations in presentations at research conferences (AIChE, ACS Colloids) and for publication in research journals

Collaboration Pharmaceuticals, Inc. — Raleigh, NC

Internship in Computational Drug Design and Machine Learning — May 2023 – August 2023

- **Curated and standardized large chemical datasets** from internet sources, like PubCHEM, ChEMBL, and the CDC
- **Used machine learning algorithms to build QSAR models**, which predict the activity of compounds against a target compound based on their chemical structures
- Applied machine learning models to: 1) virtually screen large chemical libraries for chemical hits, and 2) design novel anti-malarial compounds with generative AI software MegaSyn
- **Developed a unique application of near-term quantum computing algorithms** to cheminformatics and computational drug design problems in collaboration with team of researchers from various backgrounds
- Developed software application for building quantum QSAR models with Fujitsu *qulacs* quantum simulation package, and applied software on Fujitsu quantum simulation supercomputer

SKILLS

Languages: English (Fluent, Native Speaker), German (Level B1/2 - Conversational Fluency and Business Proficiency)
Programming Languages: Fortran 90/95, Python, bash, Java, MATLAB, C/++
HPC Schedulers: LSF (Hazel – NCSU), SLURM (Fujitsu Quantum Simulator), HTCondor (Open Science Grid)

EDUCATION

Ph.D. in Chemical Engineering Expected: May 2024

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

Working Dissertation Title: "Phase Diagrams for Systems of Magnetically-Polarized Colloids Under the Influence of External Fields"

M.S. in Chemical Engineering Dec 2021

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

Cumulative GPA: 3.56/4.00

B.S. in Chemical Engineering, Minor in Applied Mathematics Dec 2017

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

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

SELECTED PUBLICATIONS AND PRESENTATIONS

Publications

- **Dorsey, M.A.**, Dsouza, K., Urbina, F., Ranganath D., Ekins, S. (2023). *Application of Near-Term Quantum Computing Algorithms in Cheminformatics and Computational Drug Design.* (In Preparation)
- **Dorsey, M.A.**, Harris, J., Urbina, F., Ekins, S. (2023). *Generative Design of Novel Anti-Malarial Compounds with Predicted Activity against* Plasmodium falciparum. (In Preparation)
- **Dorsey, M.A.**, Hall, C.K. (2023). *Extension of Molecular Dynamics Simulations to Magnetic Ensembles with a Stochastic External Field.* (In Preparation)
- **Dorsey, M.A.**, Velev, O.D., Hall, C.K. (2023). *Computational Investigation of the Structure Properties of Colloidal Microcubes with Offset-Magnetic Dipoles in Two Dimensions*. *Soft Matter*, 2023, 19 (22), 4123 - 4136.

Conference Presentations

- **Dorsey, M. A.**, Hall, C. K. *Metastability of Colloidal Squares with Offset Dipoles at High Densities*. American Institute of Chemical Engineers (AIChE) Conference in Orlando, FL, Nov. 2023. (Accepted)
- **Dorsey, M. A.**, Hall, C. K. *Directed Assembly of Dipolar Rods in the Presence of an External Field*. American Institute of Chemical Engineers (AIChE) Conference, Orlando, FL, Nov. 2023. (Accepted)
- **Dorsey, M. A.**, Hall, C. K. *Computational Studies of the Directed Assembly of Dipolar Rods in the Presence of an External Field*. ACS Colloids and Surface Science Symposium, Raleigh, NC, Jun. 2023.

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 *(Lecturer: Dr. Erik Santiso)* and Chemical Engineering Process Principles *(Lecturers: Drs. Michael Dickey, Lisa Bullard, Milad Abolhassani)*
- 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

R. Chris Estridge

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

(Address) 361 The Greens Circle, Apt. 425, Raleigh, NC 27606

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

OBJECTIVE

Hardworking and team-oriented Chemical and Biomolecular Engineering Ph.D. candidate with diverse research experience modeling neurodevelopment and neurodevelopmental diseases with a focus on developing innovative tools to explore these systems. I aspire to join a multidisciplinary team in a technical and commercial hybrid role to leverage my technical abilities and critical thinking skills to discover creative business solutions.

RESEARCH EXPERIENCE

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

- Developing high resolution spatial transcriptomics system to improve analysis of mammalian tissue samples
- Investigating the role of Matrigel delivery methods and dosage in human cerebral organoid growth and development to improve the cerebral organoid model
- Studying developmental effects of *UBE3A* absence in human cerebral organoids to gain insight into cell-type specific outcomes of Angelman syndrome by utilizing bioinformatics tools

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

PhD Leadership Program Intern, BASF Corporation, Wyandotte, MI (May 2023 – Aug. 2023)

- Developed workflows to automate exportation and processing of data resulting in an estimated annual time savings of 500 hours.
- Led collaborative project with diverse international team of 6 people to create process flow diagrams for product registration to assist implementation of new product definition sheet system.

ChemE Co-op, 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

SELECTED LEADERSHIP AND SERVICE ACTIVITIES

- CO_2 Cell Culture Incubator and Liquid Nitrogen Storage System Equipment Manager (Aug. 2020-Present)
  - Identified safety hazards and wrote SOPs for proper equipment usage to mitigate risks
  - Managed trainings and organized sterilizations for 15 lab members
- Soccer Coach at North Carolina Football Club, Raleigh, NC (Aug. 2021-Present)
  - Coach for U15 Girls team
  - Mentors players and leads training sessions
- Undergraduate Student Lab Mentor (Jan. 2021-May 2023)
  - Managed projects and goals and provides mentorship for four undergraduate students
- Chemical Engineering Summer Camp Counselor (Jun. 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 (Jul. 2019-Jun. 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

AWARDS AND HONORS

North Carolina State University

- Genetics and Genomics Academy (GGA) Summer Mini Grant Recipient (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)

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 – Jul. 2015)

TECHNICAL SKILLS

- **Computer Literacy:** Microsoft Office, Microsoft Power Automate, MATLAB, R, JMP, ImageJ/FIJI, Adobe Illustrator, zUMIs, Seurat, SAMtools, Slingshot
- **Laboratory Techniques/Equipment:** Confocal Microscopy, qPCR, Mammalian Cell Culture, Single-cell RNA-Sequencing, Bioinformatics, Quantitative Data Analysis, Dynamic Mechanical Analysis, Thermal Gravimetric Analysis, Differential Scanning Calorimetry

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)

SELECTED PUBLICATIONS AND CONFERENCE PRESENTATIONS

- **R. Chris Estridge**, Jennifer E. O'Neill, Albert J. Keung, *Matrigel tunes human cerebral organoid development* (Manuscript under review)
- Thomas P. Rudibaugh, Ryan W. Tam, **R, Chris Estridge**, Albert J. Keung, *Single cell assessment of human stem cell derived mesolimbic models and their responses to substances of abuse* (Manuscript submitted for publication)
- **R. Chris Estridge**, Z. Begum Yagci, Dilara Sen, Jeremy M. Simon, Albert J. Keung, *UBE3A loss broadly impacts the composition and cell-type specific gene expression of human cerebral organoids* (in preparation)
- **R. Chris Estridge**, Z. Begum Yagci, Dilara Sen, Jeremy M. Simon, Albert J. Keung, *Single-Cell RNA-Sequencing Reveals Cell Type Composition Differences between Neurotypical and UBE3A Deletion Human Cerebral Organoids*, Foundation for Angelman Syndrome Therapeutics (FAST) Annual Translational Research Symposium, Hollywood, Florida (December 1-3, 2022)
- **R. Chris Estridge**, Jennifer E. O'Neill, Albert J. Keung, *Matrigel dosage regulates whole brain human cerebral organoid development*, American Chemical Society Spring Meeting, San Diego, California (March 20-24, 2022)

EDUCATION

Aug. 2018 – Present	**North Carolina State University, Raleigh, NC (Expected graduation date: June 2024)** Ph.D. Department of Chemical and Biomolecular Engineering (G.P.A.: 3.74/4.0) Thesis: *Advancing Tools to Accelerate the Study of Human Neurodevelopment*
Aug. 2018 – May 2021	**North Carolina State University, Raleigh, NC** M.S. Department of Chemical and Biomolecular Engineering (G.P.A.: 3.74/4.0)
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 (Aug. 2019-Present)
- American Chemical Society (Jan. 2022-Present)

Zach Hetzler

2236 Long Pine Lane, Raleigh, NC, 27603
252.675.3900
zjhetzle@ncsu.edu

PROFESSIONAL SUMMARY

Highly motivated current Ph.D. candidate and biotechnology professional with broad experience across analytical and biomanufacturing disciplines. Collaborative team player with strong relationship building, leadership, and communication skills. Experienced with viral vector analytical techniques, assay development, optical molecular detection systems, and technical writing and communication. Proven ability to effectively design and execute experiments, troubleshoot experimental methods and instrumentation, as well as lead teams through complex cross-functional projects.

EDUCATION

North Carolina State University, Raleigh, NC

Ph.D., Chemical & Biomolecular Engineering — Expected: 2024
M.Sc., Chemical & Biomolecular Engineering — May 2020
B.S., Human Biology — Aug 2013

PROFESSIONAL EXPERIENCE

Graduate Research Assistant

North Carolina State University, Chemical and Biomolecular Engineering, Raleigh, NC — Aug 2020 – Present

- Developed CRISPR Diagnostics-based Adeno-Associated Virus (AAV) titration assay with sample to result time of only 30 minutes, significantly reducing assay time compared to current similar molecular diagnostic methods.
- Developing microfluidic format for executing digital CRISPR (dCRISPR) assay for absolute determination of AAV genomic titer at the single molecule level.
- Developed and optimized multiple nucleic acid amplification tests including qPCR and LAMP.
- Authored research proposal resulting in $500,000 funding and collaborative team including large industry and start-up partners for development of novel gene therapy process analytical technology.
- Developed new optical carbon dioxide sensor for cell culture monitoring in bioreactors, enabling real-time and in-line process monitoring and control.
- Developed and executed methods and protocols for numerous experiments including enzymatic analysis via Michaelis-Menten kinetics, stability studies, protein/DNA titration, and absorbance and fluorescence based plate reader assays.
- Supervised 7 masters and undergrad students conducting research in our lab.
- Communicated research through oral presentations at conferences as well as an invited talk at an NC Biotech symposium.

Graduate Research Assistant

North Carolina State University, Chemical and Biomolecular Engineering, Raleigh, NC — August 2019 – May 2020

- Optimized the performance of innovative peptide ligand chromatographic resin for mAb purification operating in flowthrough mode with results comparable or better than commercially available polishing resins.
- Employed analytical techniques to quantify performance, such as Protein A (yield), Size Exclusion Chromatography (purity and aggregation quantification), and HCP ELISA (orthogonal purity determination).
- Operated solid-phase peptide synthesizer to generate peptide resin for use in dynamic binding studies.

Small Scale Fermentation Laboratory Manager – Bioprocess Training Associate — February 2017- August 2019

North Carolina State University, BTEC, Raleigh, NC

- Taught fundamentals of microbial fermentation, optimization of protein expression, and upstream scale-up parameters.
- Instructed students in the use of several molecular biology skills, such as cloning, gel electrophoresis, PCR, UV/Vis Spectrophotometry, among others.
- Instructed laboratories and employee training for academic and professional development programs for employees at organizations such as Merck, Pfizer, and the FDA.

Manufacturing Sciences Associate August 2016 – January 2017

Seqirus (formerly Novartis Vaccines), Holly Springs, NC

Part of a cross-functional team to support the tech-transfer of an enhanced flu vaccine cell culture production process aimed to meet pandemic supply commitments and significantly improve seasonal yields for commercial production.

- Led root cause analysis (RCA) teams for protocol deviations arising from engineering run errors by employing 5 whys, fishbone diagrams, as well as other RCA analysis tools.
- Assisted with authoring of the Downstream engineering run summary report by trending unit op performance and
- Collaborated with multidisciplinary teams to implement new technical procedures.
- Saved $218,000 in raw materials by authoring hold time study interim report to extend the expiry of batches of media

Downstream Manufacturing Associate March 2014 – August 2016

Seqirus (formerly Novartis Vaccines), Holly Springs, NC

- Led purification areas through process prioritization, troubleshooting, and leading associates' activities and training
- Collaborated with development engineers during tech transfer to manufacturing and assisted with development and implementation of new manufacturing operations.

PUBLICATIONS

- **Hetzler, Z**.; Lott, N.; Mohammad, N.; Lass-Napiorkowska, A.; Turrentine, L.; Fields, D.; Overton, L.; Rammo, O.; George, H.; Wei, Q.; Rapid Adeno-associated virus genome quantification with amplification-free CRISPR-Cas12a. Manuscript under preparation
- Wang, Y.; Sadeghi, S.; Paul, R.; **Hetzler, Z.**; Danilov, E.; Ligler, F.; Wei, Q..; Low-Rate Smartphone Videoscopy for Microsecond Luminescence Lifetime Imaging with Machine Learning. *PNAS* (under review)
- **Hetzler, Z.**; Wang, Y.; Krafft, D.; Jamalzadegan, S.; Overton, L.; Kudenov, M., Ligler, F.; Wei, Q. Flexible sensor patch for continuous carbon dioxide monitoring . *Front. Chem.* 2022. DOI: 10.3389/fchem.2022.983523
- Lavoie, R.A.; Chu, W.; Lavoie, J.H; **Hetzler, Z.;** Williams, T.I.; Carbonell, R.; Menegatti, S. Removal of host cell proteins from cell culture fluids by weak partitioning chromatography using peptide-based adsorbents. . *Sep. Purif. Technol.* 2021. DOI: 10.1016/j.seppur.2020.117890

LEADERSHIP/SERVICE ACTIVITIES

NSF I-corps Team Lead 2021, 2023

Led teams through regional Innovation corps (I-corps) program at NC State aimed to advance commercialization of research discoveries for two technologies from our lab. We interviewed 40+ potential customers across both programs to identify market-fit and technology needs in the commercial space. Our team was awarded $3,000 to continue commercialization efforts.

Teaching Assistant 2019 - 2022

Reaction Kinetics/Reactor Design
Chemical Engineering Analysis
Transport Processes

Professional Development Chair August 2021 – August 2022

NCSU CBE Graduate Student Association

Organized over 10 professional development seminars and workshops including a networking event with BASF attended by over 100 students and faculty as well over 20 BASF professionals ranging from manufacturing to the R&D president.

BioLunch 2022 Student Organizer May 2022 – August 2022

Assembled, organized, and introduced 3 technical presentations each week as part of a 3 student organizer team attended by graduate students from several departments aimed at giving graduate students technical presentation experience.

Head Basketball Coach January 2015 – 2017

Alexander Family YMCA, Raleigh, NC

- Managed youth ages 9–11 while instilling principles of integrity, dedication, positive self-image, and teamwork

Parenteral Drug Association (PDA) December 2016 - Present

Habitat for Humanity Active Builder November 2015 - Present

Habitat for Humanity of Wake County

ADDITIONAL SKILLS

Computers: Origin Lab, Unicorn Äkta Control Software, basic Python/Matlab coding experience

Haeleen Hong

Chemical and Biomolecular Engineering, North Carolina State University
Tel: 919-412-2011
E-mail: hhong5@ncsu.edu

RESEARCH INTERESTS

My main research interest is centered around novel **colloidal systems**, such as soft dendritic microparticles, or dendricolloids. These materials can be employed as environmentally benign **micro-cleaners** for removing microplastics and oil from water, or as ionically conductive hydrogels for **hydrogel sensors** embedded with dendricolloid fibrillar networks.

EDUCATION

Aug. 2020-present **North Carolina State University, NC, USA**

Ph. D. candidate in Chemical and Biomolecular Engineering.
Advisor: **Prof. Orlin D. Velev**

Mar. 2018– Jun. 2020 **Sungkyunkwan University, Suwon, Korea**

Researcher in School of Chemical Engineering.
Advisor: **Prof. Tae-il Kim**, Multifunctional Soft-Electronics Laboratory

Mar. 2016– Feb. 2018 **Sungkyunkwan University, Suwon, Korea**

M.S. degree in School of Chemical Engineering
Advisor: **Prof. Tae-il Kim**, Multifunctional Soft-Electronics Laboratory

Mar. 2012–Feb. 2016 **Sungkyunkwan University, Suwon, Korea**

B.S. degree in School of Chemical Engineering

EXPERIENCE

Jan. 2021-present **EFRI: Engineering the Elimination of End-of-life Plastics (NSF)**
Researcher: I have developed a new cleanup system for microplastic remediation in the ocean. This system is cost-effective, requires less energy, and is biocompatible. This project was a collaboration with Dr. C. Hall, Dr. N. Crook, and Dr. O.D. Velev at NCSU, as well as Dr. F. You and Dr. N. Abbott at Cornell.

Mar. 2017-Feb. 2018 **NANO-Convergence 2020 Program**
Researcher: Conducted research for the promotion of commercialization of research outcomes obtained from R&D activities.
Theme: High thermal conductive and flexible interface adhesive sheet using multi-layered ceramic nanocomposite.

Dec. 2015–Feb. 2016 **Linkoping University at Campus Norrkoping, Sweden**
Visiting student: Learned and understood the fabrication techniques for organic electronics such as conducting polymers as energy material in thermo-electronics in the laboratory of Prof. Xavier Crispin.

Aug. 2015-Dec. 2015 **Sungkyunkwan University, Suwon, Korea**

Undergraduate research student: Conducted research in unconventional lithography and high thermal conductive composite in the laboratory of Prof. Tae-il Kim.

HONORS AND AWARDS

Fall. 2019	**Outstanding poster presentation award** at 2019 The Korean Institute of Chemical Engineers Fall Meeting
Fall. 2015	**Excellence Manpower Training Scholarship** in Sungkyunkwan University
Fall. 2014	**Excellence Manpower Training Scholarship** in Sungkyunkwan University
Spring. 2012 - Spring. 2013	**The National Scholarship for Science and Engineering** in Korea Student Aid Foundation (KOSAF)

PUBLICATIONS

(1) **H. Hong**, R.S. Bang, L. Verster, and O.D. Velev*, "Self-propelling and dispersing active microcleaners for recovery of microplastics dispersed in water" (*Manuscript in progress)***.**

(2) W, Jung, G.R. Koirala, J.S. Lee, J.U. Kim, B. Park, Y.J. Jo, C. Jeong, **H. Hong**, K. Kwon, Y.S. Ye, and J. Kim, and T. I.Kim*, "Solvent-assisted filling of liquid metal and its selective dewetting for the multilayered 3D interconnect in stretchable electronics" ***ACS nano***, 16, 21471-21481 (2022).

(3) H. Ryu, H. Choi, J.H. Shin, **H. Hong**, B. Park, E.G. Lee, and T.I. Kim*, "Non-yellowish and heat-resistant adhesive for a transparent heat sinking film" ***Journal of Industrial and Engineering Chemistry*** *103*, 275-282 (2021).

(4) K.Y. Kwon, S. Cheeseman, A. Frias-De-Diego, **H. Hong**, J. Yang, W. Jung, H. Yin, B.J. Murdoch, F. Scholle, N. Crook and E. Crisci, M.D. Dickey*, V.K. Truong*, T.I. Kim* "A Liquid metal mediated metallic coating for antimicrobial and antiviral fabrics" ***Advanced Materials*** 33, 2104298 (2021)

(5) S.J. Kang, **H. Hong**, C. Jeong, J.S. Lee, H. Ryu, J.H. Yang, J.U. Kim, Y.J. Shin and T.I. Kim*, "Avoiding heating interference and guided thermal conduction in stretchable devices using thermal conductive composite islands" ***Nano Research*** 14, 3253-3259 (2021)

(6) J. U. Kim, S.J. Kang, S. Lee, J. Ok, Y.J. Kim, S.H. Roh, **H. Hong,** J.K. Kim, H. Chae, S. J. Kwon*, T. Kim*, "Omnidirectional, broadband light absorption in a hierarchical nanoturf membrane for an advanced solar-vapor generator" ***Advanced Functional Materials*** 30, 202003862 (2020)

(7) **H. Hong,** Y. H. Jung, J. S. Lee, C. Jung, J. U. Kim, S. Lee, H. Ryu, H. Kim, and T. Kim*, "Anisotropic thermal conductive composite by guided assembly of boron nitride nanosheets for flexible and stretchable electronics" ***Advanced Functional Materials*** 29, 1902575 (2019)

(8) S. Lee†, G. Hwang†, T. H. Kim†, S. J. Kwon, J. U. Kim, K. Koh, B. Park, **H. Hong**, K. J. Yu, H. Chae, Y. Jung*, J. Lee*, and T. Kim*, "On-demand drug release from gold nanoturf for a thermo- & chemo-therapeutic esophageal stent" ***ACS Nano*** 12, 6756 (2018) **[†equal contribution]**

(9) B. Park, S. Lee, H. Cho, J. U. Kim, **H. Hong**, C. Jeong, D. Kang* and T. Kim*, "A Semi-Permanent and Durable Nanoscale Crack based Sensor by On-Demand" ***Nanoscale*** 10, 4354-4360 (2018)

(10) **H. Hong**, J. U. Kim, and T. Kim*, "Effective assembly of nano-ceramic materials for high and anisotropic thermal conductivity in a polymer-composite" ***Polymers*** 9, 413 (2017)

PATENTS

(1) T. Kim and **H. Hong**, "Polymer-inorganic composite" *PCT patent,* PCT/KR2018/003767 (2018)

(2) T. Kim, **H. Hong**, and Y. C. Kim, "Polymer-inorganic composite" *Korea patent*, 10-1808985 (2017) Granted.
Technology transfer to DAEAN Chemical Co., Ltd, Korea.

TECHNIQUES & SKILLS

Micro-Nano Fabrication Laboratory Skills	**Unconventional Lithography -** Thermal and UV Imprinting Lithography; Micromolding in Capillaries; Microcontact Printing
	Photolithography - Midas Systems MDA-400LJ aligner
	Solution-Based Fabrication for Micro- and Nano-Particles – IKA
Software Skills	**Design, Simulation and Analysis -** Rhino; COMSOL Multiphysics; Origin Pro

PALLAV K. JANI

(734)773-5755 ● pkjani@ncsu.edu ● linkedin.com/in/pallavjani

SUMMARY

Collaborative researcher with 5+ years of combined industrial and academic experience in interfacial and polymer modification, tribology, rheology, and materials development, resulting from independent and industry-sponsored projects

Experimental & Analytical Skills: Rheology & tribology of gels and coatings; Component interactions in polymer formulations – isothermal titration calorimetry (ITC), quartz crystal microgravimetry (QCM); Goniometry; Electron microscopy (SEM-EDS); Confocal laser profilometry; Thermal analysis, FTIR spectroscopy and UV-vis spectroscopy, Physical vapor deposition

Computational Skills: MATLAB, Python, GraphPad, Origin, ImageJ, COMSOL

EDUCATION

North Carolina State University — **Raleigh, NC**
Doctor of Philosophy (Ph.D.), Chemical Engineering — January 2024

University of Michigan — **Ann Arbor, MI**
Master of Science in Engineering (M.S.E), Chemical Engineering — December 2018

Institute of Chemical Technology — **Mumbai, India**
Bachelor of Technology (B.Tech.), Oils, Oleochemicals and Surfactants — May 2017

PROFESSIONAL EXPERIENCE

Contact Physics & Tribology Intern | Corporate R&D, TE Connectivity, Harrisburg, PA — June – August 2022
Tribological investigation of surface coatings for stamping tool life improvement and EMI shielding

- Identified coating failure modes by characterizing dry and lubricated friction and wear for 15+ coating formulations
- Developed performance rating matrix and down-selected 2-3 promising coating formulations for product-level testing
- Collaborated with stakeholders from two different business units across three R&D projects

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 for diesel engines with less than 10% deviation
- Led efforts to identify and model low friction technologies such as ring coating chemistries and low viscosity oils
- Translated friction reduction into fuel economy benefits (0.6-1%) via modified fuel maps of low friction technologies

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

- Identified key areas of oil loss (1.4%) 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

RESEARCH EXPERIENCE

Graduate Researcher | North Carolina State University, Raleigh, NC — September 2019 - present
Advisors: Saad Khan and Lilian Hsiao
Interfacial friction control of stiff and soft polymers by slip additives

- Demonstrated 40 – 85% friction reduction based on adhesion and load-dominant friction dissipation modes of erucamide, a slip additive, on a polymeric substrates with varying elastic moduli from hard polyolefins to soft elastomers
- Correlated friction reduction to pressure-induced changes of the erucamide coating structure
- Showcased improved haptic sensation of slip additive-coated elastomers through human trials

Thermodynamics of epoxy-metal adhesion in bisphenol A (BPA)-based epoxy can coating formulations

- Identified adhesion mechanism and structure-property relationships of epoxy resins with three model metal oxides using ITC
- Established critical role of benzene rings of epoxy resins in the entropy-driven binding to optimize adhesion

Adsorption and interactions hydrophilic finishes on slip additive-coated polymeric nonwovens

- Correlated macroscale wetting of nonwovens to the structure of hydrophilic surfactant finishes through QCM
- Developed mechanistic understanding of the slip additive-surfactant intermolecular interactions and impact on wettability

pH-dependent interactions and rheology of bio-based collagen-tannic acid hydrogel formulation

- Determined quantitative correlation between interaction enthalpy (ΔH) and hydrogel mechanical strength at different pHs
- Identified role of hydrogel hydration in weakening of collagen-tannic acid interactions using QCM

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 turbocharger compressor coking

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

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

Advisors: Paul Zimmerman and Frank Reinhold

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

- Designed lab-scale rotating dishwashing setup to quantify dirt removal under shear via a 2^3 factorial DOE testing protocol
- Distinguished 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

Surfactant assisted co-precipitation to control nanoparticle morphology

- Examined the role of surfactant type on the morphology of synthesized nanoparticle precipitates using electron microscopy
- Optimized two precursor mixing strategies – dilution and droplet mixing, to control nanoparticle shape

SELECT PUBLICATIONS & CONFERENCE PRESENTATIONS

- Sarker, P.#, **Jani, P.#** et al. "Interacting Collagen and Tannic Acid particles: Uncovering pH-dependent Rheological and Thermodynamic Behaviors" J. Colloid Interface Sci. 2023, 650, 541-552 (#co-first author)
- Adhikari, P.#; **Jani, P.#** et al. "Interfacial contributions in nanodiamond-reinforced polymeric fibers" J. Phys. Chem. B **2021**, 125, 10312-10323 (#co-first author)
- **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**

LEADERSHIP AND OTHER ACTIVITES

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

- Advanced Process Modeling (Fall 2020), Transport Phenomena (Spring 2021), Polymer Rheology (Spring 2022)
- Designed homework and examinations for graduate-level courses of process modeling and polymer rheology for 30+ students

Certificate Courses

- Absorbent Hygiene Technical Training | INDA, Association of the Nonwoven Fabrics Industry (2023)
- Python Basics | Embedded Machine Learning Club, North Carolina State University (2023)

Event Organizer | Institute of Chemical Technology, Mumbai, India

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

AWARDS & PROPOSALS

- Contributed towards drafting a successful research grant proposal on "biopolymer surface modification and biodegradability" sponsored by The Nonwovens Institute at North Carolina State University worth $180K (2022)
- 'Best Overall Award' and 'Best Technical Award' for technical and presentation excellence at The Nonwovens Institute's Industry Advisory Board Meeting for research on slip additive – surfactant coating interactions (2022-23)
- 'Division of Soft Matter Meeting Grant' to support attendance at the American Physical Society Annual Meeting (2021)
- 'Provost's Doctoral Fellowship' and 'Graduate Merit Award' (2019-2020)

GAUTAMI KELKAR

Raleigh, NC 27606 | 919-510-2850 | grkelkar@ncsu.edu | www.linkedin.com/in/gautami-kelkar/

EDUCATION

- Ph.D. student, Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, NC, 2022-Present (GPA- 3.78/4)
- MS, Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, NC (2022) (GPA- 3.78/4)
- Bachelor of Chemical Engineering, Institute of Chemical Technology, Mumbai, India (2020) (GPA 8.68/10)

TECHNICAL SKILLS

- **Cell Biology:** Cell Culture (human embryonic stem cells, iPSCs, and HEKs), 3D Organoid culture
- **Microscopy/Imaging:** Confocal microscopy, Cell and tissue imaging and analysis
- **Biochemistry:** Tissue fixation, Immunofluorescence staining, Flow Cytometry (FACs) analysis
- **Molecular biology:** PCR, Gel Electrophoresis, Sanger sequencing, Mini prep (solid tissues), Bisulfite Conversion of genomic DNA, Protein Extraction
- **Transcriptomics:** scRNA-sequencing data analysis, spatial transcriptomics
- **Programming languages:** R, Python, and Matlab
- **Software:** MS Word, Excel, and PowerPoint, Minitab, Ansys, SnapGene, ImageJ, FlowJo, CellProfiler, TECAN and GenomeStudio

RESEARCH EXPERIENCE

North Carolina State University, Department of Chemical and Biomolecular Engineering
Graduate Research Assistant with Dr. Albert Keung (https://keunglab.wordpress.ncsu.edu/) *Jan 2021- Present*

- Development of human stem-cell-derived cerebral organoids as aging and age-associated disorders models.
  - Assessed the stress response of cultured cerebral organoids to Hydrogen Peroxide exposure using immunofluorescence studies
  - Isolated DNA from organoids and performed DNA bisulfite conversion (for methylation analysis)
  - Wrote an R to analyze DNA methylation data with the epigenetic "clock" algorithms that correlate methylation and aging.
- Studying the role of metabolism in stress and cell-type composition in human brain organoids *(in progress)*
  - Measured the abundance of Reactive Oxygen Species in response to varying metabolite availability
  - Investigated the influence of metabolites on proliferation using flow cytomtery-assisted EdU assays
  - Performed immunofluorescence studies for cell type-specific biomarkers to quantify the relative proportions of each cell type
- Engineering a high-throughput tissue-compatible spatial transcriptomics system using microfluidic devices *(in progress)*
  - Trained in the fabrication of a microfluidic device mold using a silicon wafer
  - Isolated barcoded nuclei from mouse tissue sections for fixation and RNA extraction
  - Developed a post-processing workflow for extracting barcode information and spatial assignment from RNA sequencing reads using Python

ICT Mumbai
Team project *January 2018-March 2018*

- Computational Fluid Dynamics (CFD) modeling of motion of food particles due to gastric motility.
  - Used WebPlot Digitizer and SolidWorks to create the stomach geometry for simulations
  - Used Ansys 17.0 to simulate peristalsis and the motion of food particles through the stomach
  - Presented the project in a national competition at IIT Bombay and stood 1st.

IIT Bombay
Undergraduate Research Assistant *May 2018-November 2018*

- Rheological characterization of polyacrylamide gels which are used for studying cell migration *in vitro*
  - Used a rheometer to measure viscoelastic properties of polyacrylamide gels
  - Used MATLAB to model phenomenological data obtained from creep tests using the Kelvin-Voigt model

TEACHING AND LEADERSHIP EXPERIENCE

- Graduate Teaching Assistant for Design and Analysis of Chemical Reactors - Prof. Albert Keung (2021)
- Graduate Teaching Assistant for Transport Processes - Prof. Stefano Menegatti (2022)
- Student Organizer for Biolunch Graduate Seminar Series for Summer 2023

PUBLICATIONS

- **Kelkar GR***, Yagci ZB*, Johnson TJ*, Sen D*, Keung AJ; Designing Epigenome Editors: Considerations of Biochemical and Locus Specificities; Methods in Molecular Biology (accepted)

AWARDS

- NC State College of Engineering: Graduate Merit Award (2021)
- NC State CBE Department: Best Research Image Award (2023)

CONFERENCE PRESENTATIONS

Using DNA methylation analysis as a tool to develop in vitro models for human aging studies

- International Conference on Epigenetics and Bioengineering (EpiBio) 2021: Poster presentation
- Synthetic Biology: Engineering, Evolution & Design (SEED) 2022: Poster presentation and Rapid Fire talk

Investigating the role of metabolism in human stem cell differentiation and development using organoid models

- BMES Annual Meeting 2023: Poster presentation (accepted)
- AIChE Annual Meeting 2023: Oral presentation (accepted)

Ryan Kilgore

Phone: (919) 606 9146 | Email: rekilgore1@gmail.com
Address: Raleigh, NC | LinkedIn: www.linkedin.com/in/ryankilgore1

SUMMARY

I am a 5th year Ph.D. candidate specializing in downstream biomanufacturing research, focusing on advanced purification techniques for next-generation therapeutics, such as exosomes, Fab fragments, scFv, and CRISPR Cas12a. I also bring practical leadership experience, having successfully managed a 17-member team in OTC pharmaceutical liquids manufacturing at Procter & Gamble.

EDUCATION

NORTH CAROLINA STATE UNIVERSITY — Raleigh, NC

Ph.D. Chemical Engineering - GPA 3.68 – Expected March 2024 — August 2019 – Expected March 2024

M.S. Chemical Engineering - GPA 3.68 — August 2019 – December 2021

B.S. Chemical Engineering - GPA 3.62 — August 2013 – May 2017

EXPERIENCE

NORTH CAROLINA STATE UNIVERSITY — Raleigh, NC

- ***Ph.D. Candidate – Advised by Dr. Stefano Menegatti*** — August 2019 – Expected March 2024
  - Thesis: Development of peptide-based affinity ligands for the purification of next-generation biotherapeutics.
  - **6 first/co-first author publications expected** including 1 corresponding author publication
    - Published: Development of peptide affinity ligands for the purification of polyclonal and monoclonal Fabs from recombinant fluids – DOI: 10.1016/j.chroma.2022.463701
    - Published: De novo discovery of peptide-based affinity ligands for the Fab fragment of human immunoglobulin G - DOI: 10.1016/j.chroma.2022.462941
    - Published as corresponding author: The downstream bioprocess toolbox for therapeutic viral vectors – DOI: 10.1016/j.chroma.2023.464337
    - Manuscript Completed: Peptide Ligands for the Universal Purification of Exosomes by Affinity Chromatography
    - Research ongoing: CRISPR Cas12a purification by peptide affinity ligands
    - Research ongoing: Isolation of human polyclonal IgG and scFv from *Pichia Pastoris* perfusate
  - 1-2 patents
    - One under prosecution for Fab and scFv purification
    - One not yet filed for the exosome work.
  - 8+ co-authored papers (second author or below)
    - AAV purification - Biotechnol. Bioeng. (2023); Lentivirus purification – Biotechnol. Bioeng. (2023); AAT purification – J. Chromatogr. A (2023); Review on peptide affinity ligands - J. Chromatogr. A (2021); Lyopreservation of *Clostridium ljungdahlii* - Plos One (2017). Ongoing efforts: AAV purification, Adenovirus purification, and light responsive peptides.
  - Research Experience
    - Extensive purification experience of exosome, Fab fragment, CRISPR Cas nuclease, and IgG from HEK293, CHO-S, *E. coli*, and *Pichia Pastoris* fluids. Some experience with AAV, Lentivirus, AdV, and scFv purification.
    - Skilled in the use of ÄKTA chromatography systems and HPLC systems (Waters, Agilent, and ThermoFisher) for purification and analysis of proteins using affinity chromatography (with both custom adsorbents and commercialized adsorbents (e.g., Cytiva MabSelect SuRe)) size exclusion chromatography (SEC), and ion-exchange chromatography (IEX), with some experience in reverse phase (RP), mixed mode (MMC), hydrophobic interaction (HIC), and steric exclusion chromatography (SXC).
    - Skilled in techniques for protein analysis: quantification with BCA and Bradford assays; purity determination with ELISA and SDS-PAGE; peptide analysis via Edman Degradation; particle size and count by multi-angle light scattering (SEC-MALS) and nanoparticle tracking analysis (NTA).
    - Cell culture experience: a *Pichia Pastoris* continuous perfusion fermentation system started from agar stab and glycerol stock, to expansion with shake flasks and production in 500 mL bioreactor; *E. coli* lysate preparation from plate to shake flask; and HEK293 production from frozen stock to shake flask.
    - Organic chemistry experience: Solid phase peptide synthesis via Fmoc/tBu chemistry.
  - Oral Presentations
    - ACS Spring 2022, PREP 2022, Affinity 2023, ISPPP 2023, AIM-Bio symposium (2021, 2022, 2023)

PROCTER & GAMBLE — Greensboro, NC

- ***Line Leader – Bulk liquid production of FDA regulated, OTC pharmaceuticals*** — September 2018 – August 2019

Ryan Kilgore

Phone: (919) 606 9146 | Email: rekilgore1@gmail.com
Address: Raleigh, NC | LinkedIn: www.linkedin.com/in/ryankilgore1

- **Managed 17 direct reports** in the liquids manufacturing department.
- Owned the liquids manufacturing results for NyQuil, DayQuil, and ZzzQuil including production, quality, cost, delivery, safety, and morale. Assisted with Pepto Bismol active pharmaceutical ingredient (API) production.
- 45% reduction in unplanned downtime (UPDT) YOY, 75% reduction in UPDT impacts to customer YOY, 55% reduction in scrapped batches YOY, and 53.7% reduction in Quality Deviations YOY.

- ***Process Engineer*** June 2017 – September 2018
  - **Top-10% rated engineer within my ranking cohort** noted for high performance, delivering results, and being able to effectively collaborate with other people and teams (e.g., Quality Assurance). Received a rapid promotion to line leader.
  - Served as the technical resource for delivering base production needs, resolving quality deviations, and owning engineering projects for the liquids manufacturing department making Pepto Bismol, NyQuil, DayQuil, and ZzzQuil.

- ***Technical Engineering Intern*** May 2016 – August 2016
  - Specified and ordered >$32,000 worth of equipment, developed engineering documents, hired engineering consultants and contractors, refined quotes, assisted in driving the site's sustainability programs

PARKER HANNIFIN (PREVIOUSLY LORD CORPORATION) Cary, NC

- ***Technical Sales Representative Intern – Industrial Adhesives*** January 2015 – August 2015
  - Researched new market opportunities, provided recommendations for territory managers, and converted leads
  - My percent conversion of cold leads to warm leads was 4x the running average.

NC STATE UNDERGRAD RESEARCH Raleigh, NC

- ***Undergraduate Research Assistant in Dr. Michael Flickinger's Group*** January 2015 – December 2015
  - Worked on gas-to-liquid biofuel production by helping to stabilize large numbers of dry cells on bioreactor modules.
  - Recipient of a $1,000 undergraduate research grant that helped fund my research.
  - 5th author on a PLOS ONE published article.

ACTIVITIES

SUSTAINABILITY FUND ADVISORY BOARD Raleigh, NC

- ***Chairman of the Board*** August 2015 – May 2017
  - Oversaw a ten-member board (6 students and 4 faculty/staff) that distributed **$341,000** to 28 sustainability related projects, education, and resources that enhanced campus and student learning.

NC STATE STEWARDS Raleigh, NC

- ***Project Manager*** August 2013 – May 2017
  - Awarded a $30,000 grant to implement solar solutions to increase student's ability to study and lounge outside.
  - Orchestrated three Energy and Water Challenges that involved ~2000 students and saved NCSU $13,500.

NET IMPACT Raleigh, NC

- ***President & Consultant*** August 2014 – May 2017
  - Presided over the activities of our chapter. Consulted with local companies to help them pursue B Corp Certification.

Joseph Koelbl

Raleigh, NC 27591 | (256) 509-8807 | jmkoelbl@ncsu.edu

EDUCATION

Iowa State University Ames, IA
B.S. in Chemical and Biological Engineering, GPA: 3.65 May 2018

North Carolina State University Raleigh, NC
M.S. and PhD Chemical and Biological Engineering, GPA: 3.62 Expected May 2024

RELATED COURSEWORK

- Graduate Chemical Engineering Process Modeling
- Graduate Reaction Engineering and Fluid Dynamics
- Graduate Thermodynamics
- Confocal Microscopy
- Biological Dynamics: from Molecules to Organisms

RESEARCH EXPERIENCE

North Carolina State University Raleigh, NC
Graduate Research Assistant Jan 2019 -Present

- Managed junior level graduate and undergraduate students to drive research projects forward toward publication.
- Managed day to day upkeep of the research lab and maintained safety protocols and plans for the lab.
- Developed python codes for PDE mathematical modeling of cell migration and model output analysis.
- Initiated and completed a plan to establish an incubator for our microscope out of multiple environmental controllers and chamber components to improve long term cell viability.
- Improved techniques in synthetic biology, microscopy, sterile cell culture, and microfluidics.
- Mastered techniques in fluorescent microscopy especially total internal reflection fluorescence.
- Assisted in the production of microfluidic platforms for long term chemical gradients and rapid printed gradients for cell migration experiments.

Hudson Alpha Research Institute Huntsville, AL
BioTrain Summer Internship May 2017 – Aug 2017

- Improved a microfluidic model organ for further research of chronic kidney disease.
- Interfaced with research lab and startup for development of the model organ platform.
- Developed skills in microfluidics and cell culture including primary cell lines.

Iowa State University Ames, IA

Griswold Undergraduate Research Intern May 2016 – May 2018

- Learned skills in cell culture and fluorescent microscopy.
- Spearheaded analysis for several publications of a senior level graduate student.

SKILLS

- Python Image Analysis
- Python Mathematical Modeling
- Matlab
- Cell Culture
- Synthetic Biology Techniques
- Fluorescent Microscopy
- Microfluidics

Publications

Second Authorship:

Scott A. Baldwin, Shawn M. Van Bruggen, Joseph M. Koelbl, Ravikanth Appalabhotla, James E. Bear, Jason M. Haugh; Microfluidic devices fitted with “flowver” paper pumps generate steady, tunable gradients for extended observation of chemotactic cell migration. Biomicrofluidics 1 July 2021; 15 (4): 044101

Wang J, Boddupalli A, Koelbl J, Nam DH, Ge X, Bratlie KM, Schneider IC. Degradation and Remodeling of Epitaxially Grown Collagen Fibrils. Cell Mol Bioeng. 2019 Feb;12(1):69-84.

Juan Wang, Joseph Koelbl, Anuraag Boddupalli, Zhiqi Yao, Kaitlin M. Bratlie, Ian C. Schneider, Transfer of assembled collagen fibrils to flexible substrates for mechanically tunable contact guidance cues, Integrative Biology, Volume 10, Issue 11, November 2018, Pages 705–718

NOOR MOHAMMAD

Graduate Research Assistant (Wei Group)
Department of Chemical and Biomolecular Engineering, NC State
Address: 2814-21 Brigadoon Drive, Raleigh, NC 27606, USA
Contact: 919-744-8941, Email: nmohamm3@ncsu.edu

FIELDS OF INTEREST

Biosensors; Point-of-care detection; CRISPR-Dx; Microfluidics; Liquid biopsy, Cancer, and Cytotoxicity

EDUCATION

2024 (Tentative)	Ph.D. (5^{th} year running)	Chemical and Biomolecular Engineering, NC State University (Advisor: Qingshan Wei)
2018	M.Sc. **(CGPA 4/4)**	Chemical Engineering, Bangladesh University of Engineering and Technology (BUET), Dhaka (Advisor: Shoeb Ahmed)
2016	B.Sc. **(Gold Medalist, Rank # 1/78, highest CGPA in Engineering Faculty)**	Chemical Engineering, Bangladesh University of Engineering and Technology (BUET), Dhaka (Advisor: M. A. A. Shoukat Choudhury)

POSITIONS

Jun 2019 - Aug 2019	Assistant Professor, Chemical Engineering, BUET, Dhaka
Apr 2016 - Jun 2019	Lecturer, Chemical Engineering, (BUET, Dhaka

AWARDS & HONORS

Vivian T. Stannett Fellow for Outstanding Early Publication, CBE, NC State University 2023
Finalist, Linde Exceptional Teaching Assistant Award, CBE, NC State University, Spring 2021
Provost's Doctoral Fellowship, NC State University, Fall 2019 through Summer 2020
Bangladesh-Sweden Trust Fund (BSTF) Scholarship, 2020
Prestigious Prime Minister Gold Medal Award, 2018
Dean's list Award, Dept. Merit List Scholarship, and Technical Scholarship, BUET; All academic sessions
Imdad Sitara Khan Scholarship, 2008-09; Babylon Scholarship, 2008-09; Junior Scholarship Award, 2005; etc.

SKILLS AND EXPERTISE

Excel VBA, C++, Python 3.8, MATLAB, Aspen HYSYS, AutoCAD, AI 2019, Photoshop 7.0, Biorender, etc.
Skill in using Electron Microscope, 3D printing system, Microchip fabrication system, Micro array printer, PCR machine, GC, Spectrophotometer, Plate reader, Nanodrop, Mammalian Cell Culturing Equipment, etc.

PROFESSIONAL EXPERIENCES

Teaching and TAing:
Courses taught at BUET: CHE 202 (Material and Energy Balance), CHE 308 (Chemical Process Analysis), CHE 310 (Computational Technique in Chemical Engineering), CHE 402 (Fuel Analysis).
Courses TAing at NC State: CHE 205 (Chemical Process Principles), CHE 225 (Introduction to Chemical Engineering Analysis), CHE 717 (Chemical Reaction Engineering)
Consultancy: Worked as co-consultant under the project 'Resource Efficient Cleaner Production (RECP) in South Asia Region Baseline Study' offered by World Bank, 2017

SHORT COURSES, TRAININGS AND WORKSHOPS

Instructor, Staff training under Higher Education Quality Enhancement Project, ChE dept. BUET, 2018
Course on 'Biosafety and Mammalian Cell Culture' at University of Dhaka, 2017
Trainee, 'Foundation Training for Newly Appointed Faculty Members' workshop organized by BUET, 2017

PROFESSIONAL ACCREDITATION AND ASSOCIATION

Member, Biomed. Eng. Soc. (BMES), American Inst. of Chem. Eng. (AIChE), American Chem. Soc. (ACS)

INDUSTRY VISITS/EXPERIENCES

R&D support at Renata LTD, Dhaka 2015-2016, Internship at Kailastila Gas Field, Sylhet, 2015

ORGANIZATIONAL ACTIVITIES AND LEADERSHIP QUALITY

Officer, CBE-GSA (Professional development chair), NC State (August 2023-present)
Lab manager, Wei research group, CBE dept. NC State University, 2020-present
Volunteer, Graduate recruiting weekend events, CBE dept. NC State University, 2023
Member, Board of undergraduate studies (BUGS), ChE dept. BUET 2016-2019
Selected Student speaker, Prime minister gold medal award ceremony, 2018
Member and proofreader, 5th International conference on chemical engineering, Dhaka, Bangladesh, 2017
Team Member, B.Sc. course curriculum development, and B.Sc. lab manual preparation; BUET, 2017-18
Member, '100-member youth delegation of Bangladesh to India', to meet honorable president of India, 2015.

PUBLICATIONS

I. Journal Articles (* Corresponding author, † Equal contribution**)**

1. S. Jamalzadegan, S. Kim, **N. Mohammad**, H. Koduri, Z. Hetzler, G. Lee, M. D. Dickey*, Q. Wei*. Liquid Metal-Based Biosensors: Fundamentals and Applications. ***Adv. Funct. Mater.*** (Under review)
2. **N. Mohammad**, L. Talton, Z. Hetzler, M. Gongireddy, Q. Wei*. Unidirectional Trans-Cleaving Behavior of CRISPR-Cas12a Unlocks for an Ultrasensitive Assay Using Hybrid DNA Reporters Containing a 3' Toehold. ***Nucleic Acids Res.*** 2023, gkad715.
3. T. Shymanovich, A. Saville, **N. Mohammad**, Q. Wei, D. Rasmussen, K. Lahre, D. Rotenberg, A. Whitfield, and J. Ristaino*. Disease progress and detection of a California resistance breaking (RB) strain of tomato spotted wilt virus (TSWV) in tomato with LAMP and CRISPR-Cas12a assays. ***PhytoFront***. (in press)
4. Z. Weng†, Z. You†, J. Yang, **N. Mohammad**, M. Lin, Q. Wei, X. Gao*, Y. Zhang*. CRISPR-Cas Biochemistry and CRISPR-Based Molecular Diagnostics. ***Angew. Chem. Int. Ed.*** 2023, e202214987.
5. **N. Mohammad**, S. S. Katkam, and Q. Wei*. A Sensitive and Nonoptical CRISPR Detection Mechanism by Sizing Double-Stranded λ DNA Reporter. ***Angew. Chem. Int. Ed.*** 2022, e202213920.
6. **N. Mohammad**, S. S. Katkam, and Q. Wei*. Recent Advances in Clustered Regularly Interspaced Short Palindromic Repeats-Based Biosensors for Point-of-Care Pathogen Detection. ***CRISPR J.*** 2022, 5, 500-516.
7. L. A. Stanciu*, Q. Wei, A. K. Barui, and **N. Mohammad.** Recent Advances in Aptamer-Based Biosensors for Global Health Applications. ***Annu. Rev. Biomed. Eng.*** 2021, 23, 433-459.
8. **N. Mohammad**, S. Sikder, M. S. I. Bhuiyan, S. Ahmed*. Comparative Assessment of Growth and Morphological Responses Reveals Resilience of HeLa cells over Vero Cells on Exposure to Arsenic (III). ***AJPHS***, 2020, 10(2), 2291-2302.

II. Conference Proceedings

1. **N. Mohammad**, S. Sikder, M. S. I. Bhuiyan, S. Ahmed, "Cellular Responses to Arsenic Exposure Leading to Different Carcinoma", *ICCHE* 2017, p169-176.
2. M. N. Sakib, **N. Mohammad**, N. Barua, M. R. Amin, "Flow Sheet Development and Simulation with Optimization of Industrial Scale Natural Gas Processing Plant by Using Aspen-Hysys", *ICMIME* 2015, p84.

III. Dissertations

1. **N. Mohammad**, "Cytotoxic Effect of Arsenic on the Growth and Morphological Responses of Mammalian Cells'", Thesis for M.Sc. Degree, Supervisor: Dr. Shoeb Ahmed, ChE Dept., BUET, 2018.
2. **N. Mohammad**, S. Barua, "Biogas Production from Kitchen Waste in Batch and Continuous Process", Thesis for B.Sc. Degree, Supervisor: Dr. M. A. A. Shoukat Choudhury, ChE Dept., BUET, 2016.
3. **N. Mohammad**, M. N. Sakib, R. Bashar, S. Barua, "Design of a 100 Tonnes/Day Bioethanol Production Plant from Corn Starch", Supervisor: Dr. Shoeb Ahmed, ChE Dept., BUET, 2016.

CONFERENCE/ SEMINAR PRESENTATIONS

1. **N. Mohammad**, L. Talton, Z. Hetzler, M. Gongireddy, Q. Wei, "Preferential Trans-Cleaving Behavior of CRISPR-Cas12a Towards 3'-Overhang dsDNA Unlocks to Develop Ultrasensitive Hybrid DNA Reporter", ***2023 AIChE Annual Meeting***, Orlando, FL, Nov 6, 2023.
2. **N. Mohammad**, L. Talton, S. Dalgan, Q. Wei, "CRISPR-Cas12a-Induced DNA Supercoil Relaxation for Nonfluorescent Ratiometric DNA Detection", ***2023 BMES Annual Meeting***, Seattle, WA, Oct 13, 2023.
3. **N. Mohammad**, "CRISPR-Cas12a-induced unidirectional trans-cleaving of dsDNA substrate with overhang", BioLunch Seminar Series, NC State University, June 14, 2023. (Seminar)
4. **N. Mohammad**, S. Katkam, Q. Wei, "Nonfluorescent CRISPR-Cas12a Biosensor by Sizing λ DNA", *Student Competition in Sensors (Sponsored)*, ***2022 AIChE Annual Meeting***, Phoenix, AZ, Nov 14, 2022.
5. **N. Mohammad**, S. Katkam, Q. Wei, "Ultrasensitive CRISPR-Cas12a Assay Using λ DNA as Reporter Molecules", *Microfluidics/Paper-Based Diagnostics*, ***ACS Fall 2022 National Meeting***, Chicago, IL, Aug 21, 2022.
6. **N. Mohammad**, S. Sikder, M. S. I. Bhuiyan, S. Ahmed, "Cytotoxic Effect of Arsenic on the Growth and Morphological Responses of Mammalian Cells", ***AFOB***, Dhaka, 2018.
7. **N. Mohammad**, S. Sikder, M. S. I. Bhuiyan, S. Ahmed, "Cellular Responses to Arsenic Exposure Leading to Different Carcinoma", ***ICCHE***, Dhaka, 2017.

CONFERENCE POSTERS

1. **N. Mohammad**, L. Talton, S. Dalgan, Q. Wei, "Nonfluorescent Ratiometric Sensing Utilizing CRISPR-Cas12a-Induced DNA Supercoil Relaxation", ***2023 AIChE Annual Meeting***, Orlando, FL, Nov 6, 2023.
2. **N. Mohammad**, M. Gongireddy, Q. Wei. "CRISPR-Cas12a-based unidirectional trans-cleaving of dsDNA substrate with toeholds", ***ACS Fall 2023 National Meeting***, San Francisco, CA, Aug 15, 2023.

STUDENT MENTORING

4 peers (including one PhD) and 3 undergraduate students. Most of the mentees contributed as coauthors of my papers.

SNEHA MUKHERJEE

Raleigh, NC, US| +1-984-255-3376| smukhe22@ncsu.edu | Google Scholar | LinkedIn

SUMMARY

PhD student with extensive research experience in drug formulation development, wearable sweat sensors, paper microfluidics based sensors, lateral flow assays, POC devices, colorimetric and biological assays for health monitoring. PhD studies also include synthesizing DNA & RNA based nanoparticles and tuning their surface and colloidal properties. Additionally, worked on advanced 2-D materials, nanomaterials and nanofibers for supercapacitors, air filters and biomedical applications; leaching and CO_2 sequestration.

EDUCATION

North Carolina State University, Raleigh, US — **Aug'19 – Present**
PhD – Chemical Engineering — GPA:3.92/4
MS – Chemical 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

RESEARCH EXPERIENCES

'Role of selective excipients in drug formulations and their impact on product quality attributes', Drug Product Development (Steriles) — **Research Intern May-Aug'23**

- Worked with certain excipients used in formulations, performed stability studies and studied their impact on some new assets within the company.

'Well-defined, stable DNA nanoaggregates to enhance high density information storage' – funded by NSF
Advisor: Dr. Orlin D. Velev, NCSU — **PhD Candidate Aug'21– Present**

- Formulating and characterizing the surface and colloidal properties of these salt-actuated stable DNA & RNA nanoparticles and applying them towards high density and high-capacity information storage.

'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– Present**

- Developed a lateral flow assay on a wearable platform for non-invasive and zero power analyte (lactate, cortisol, potassium ions) detection in sweat. The devices are developed to be functional and effective under extremely low sweating conditions. Human trials were performed to validate patch functioning

WORK EXPERIENCES & INTERNSHIPS

- **Drug Product Development Intern, GSK, Collegeville, Pennsylvania** — May'23-Aug'23
- **'2D materials beyond graphene' (MXenes and Chalcogenides)** & **'Biomimetic Synthesis and Characterization of Nanocomposites/Nanofibers'** – Advanced Functional Materials, Council for Scientific & Industrial Research– National Metallurgical Laboratory. — Jun18–Jul'19
- **'Demineralisation of High Ash Coal'** –Tata Steel R&D Centre & IIT Kharagpur — Jun'17–Apr'18
- **'Design & 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

TECHNICAL SKILLS

- **Programming tools:** MATLAB, SCILAB, C, C++, Java.
- **Software:** ANSYS, ASPEN PLUS, UNISIM, Origin, X'Pert HighScore, GAMRY Framework, Casa XPS, ImageJ and MS Office.
- **Laboratory experience:** SEM-EDS, FTIR, XPS (analysis), XRD (analysis), TGA, Electrospinning, UV-Vis DRS analysis, Dynamic Light Scattering, Optical Microscopy, Atomic Force Microscopy, Tensile Tests, Goniometer, Differential Scanning Calorimetry, Potentiodynamic and Antibacterial tests, Assay Development and Human Trials.

SELECTED PUBLICATIONS & CONFERENCES

- **S.Mukherjee**, S.P. Salazar, T.Saha, M.D.Dickey, O.D.Velev "**Development of a Capillary-Osmotic Wearable Patch Based on Lateral Flow Assay for Sweat Potassium Analysis**", *Advanced Healthcare Materials*, under review
- 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 TiO_2 coated Fe_3O_4-SiO_2 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.
- **"Development of capillary-osmotic wearable patches for sweat analysis of potassium & cortisol via lateral flow assays"**, Oral and Poster presentations in ACS Fall 2021; ACS Colloids 2022; Triangle Soft Matter Symposium, 2021–2022; Schoenborn & MBTP Research Symposiums, Raleigh, 2021–2022.
- **"A Wearable Patch for Prolonged Sweat Lactate Harvesting and Sensing"**, 2021, 43rd Annual International Conference of the IEEE Engineering in Medicine & Biology Society (EMBC), Mexico, 6863–6866.

AWARDS & ACHIEVEMENTS

- Won the Best Poster award for "Dynamic DNA nanoaggregates while salting-in" in the Molecular Biotechnology (MBTP) Symposium in NCSU, Raleigh (March'2023)
- Awarded a Mentored Teaching Fellowship (MTF) for the Spring 2022 semester from the College of Engineering, NC State for providing teaching assistantship for CHE 596.
- Nominated twice 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 and CHE 596.
- Secured a 95.3 percentile 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)

LEADERSHIP & VOLUNTEERING EXPERIENCE

- Key organizer for the annual ACS Colloids Conference 2023 in Raleigh, NC.
- Departmental student representative and moderator on a Faculty Selection Committee for CBE, NC State for Spring'23.
- Graduate Recruiting Captain for the Department of Chemical & Biomolecular Engineering, NC State for Spring 2022. Leading the International Recruiting Event for the department in 2022 and 2023.
- Secretary & Webmaster for the Graduate Student Association, CBE, NC State for the year 2021-2022.
- Coordinator for the teams of 'School Sessions' and 'Awareness against Child Sexual Abuse' for an NGO 'Child Rights and You' (CRY) (Kharagpur, India, November'16 to May'18).

TEACHING & 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

K Himendra Perera – khperera@ncsu.edu **–** (864)-497-2179 **–** https://github.com/khperera

Education

PhD Chemical Engineering (data science emphasis) March 2024
NC State University, Raleigh, NC 3.89/4.0

B.S. Chemical Engineering (computer science emphasis) May 2019
Clemson University 3.98/4.0

Experience

PhD Candidate, Chemical Engineering January 2020 – Present
Chemical Engineering Department, NCSU Raleigh, NC

- Partnered with various industries using software engineering practices, specializing in high-performance computing and data analytics to solve complex fluid dynamics challenges.
- Led initiatives to engineer algorithms, achieving major efficiency increases in operations—tasks that previously took weeks were reduced to minutes.
- Initiated coding teams composed of graduate students, managing software and algorithm development to ensure timely and accurate project delivery.

Undergraduate Researcher January 2017 – May 2019
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.
- 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

- Led two R&D projects in consumer and industrial packaging, collaborating with operators and technicians to utilize technologies that reduce plastic usage.
- Offered a full-time position at the end of the internship in recognition of exceptional performance.

Projects

Physics Informed Neural Nets for Estimation of CO2 Diffusion Constant

- Developed a high-pressure cell for viewing and analysis of polymeric materials exposed to supercritical fluids, with a focus on renewable polymers.
- Architected and implemented a predictive neural net model using TensorFlow and DeepXDE, designed to optimize the use of limited and expensive experimental data.
- Integrated the model into a major chemical corporation's existing workflow, resulting in substantial cost savings in data acquisition and enhancing the accuracy of process simulations.

Real-Time Data Ingestion, Cleaning, and Storage for Inline Fluid Analysis

- Developed a flow cell rheometer with piezoelectric sensors integrated with analog to digital signal converter for high-frequency data capture (up to 1 MHz).
- Engineered a Python/C++ solution for real-time piezoelectric sensor data capture, achieving a 10x performance boost and implemented a modular API for seamless integration to other equipment.
- Incorporated real-time data cleaning algorithms within a streaming architecture, backed by a local SQL database, ensuring immediate and accurate fluid property analysis.
- Developed a PyQt5-based GUI to enhance user experience, promoting wider tool adoption.

Technical Project Lead for Automation and Data Integrity of ACS Conference

- Spearheaded a team responsible for data entry and validation, implementing cleaning algorithms that eliminated entry inaccuracies, a critical requirement for a conference with over 500 attendees.

- Engineered a robust testing infrastructure to systematically identify and rectify bugs and ensured data quality across multiple dimensions including scheduling and naming conventions.
- Implemented automation processes that led to a 95% reduction in manual workload, while enabling real-time modifications to event details, thereby enhancing operational efficiency.

Internet-Connected PID Controller for Polymer Extruder

- Engineered an internet-connected PID controller for a 1-ton polymer extruder, optimizing real-time control loops and implementing safety mechanisms such as overcurrent and crush protection.
- Developed a real-time monitoring GUI and ensured seamless interoperability with other process control elements for a fully integrated, automated control system.

Feature identification within Agricultural Fluids

- Gained insight into pesticide and herbicide release rates through K-means clustering and Gaussian mixture models to categorize particle clusters, which define fluid flow and help dictates pesticide release rates depending on particle density.
- Analyzed fluidic confocal microscopy data with graph theory using SciKit Image, OpenCV, and NetworkX.
- Extracted data from proprietary file formats and used XML parsing to improve data usability.

Understanding Hollow Fiber Extrusion via Computational Fluid Dynamics

- Leveraged open-source Computational Fluid Dynamics (CFD) software, including OpenFOAM and ANSYS, to design and validate extrusion dies for polymer processes, reducing prototyping costs by 75%.
- Applied CFD techniques to model 2-phase viscoelastic flows, providing critical insights that resolved discrepancies in experimental data and guided further research.
- Utilized SOLIDWORKS for the end-to-end design and stress/temperature validation of extrusion dies, confirming mechanical stability and performance under processing conditions.

Automated Video and Image Analysis with Large Amplitude Oscillatory Shear Rheology

- Implemented image processing algorithms using FIJI, SciKit Image, and OpenCV for real-time analysis of 4K video morphology in roll coating operations.
- Developed modular Python code to streamline the cleaning and Fourier-Transform analysis of rheology data in CNT composites, reducing a week's worth of analysis to minutes.
- Produced intuitive, high-quality visuals with Seaborn and Matplotlib, correlating rheology data to roll coating morphology and contributing to a manuscript submitted to a peer-reviewed journal.

Publications

1. Perera, H., Black, B., Ryu, J.E., Corder, R., Khan, S., “Ribbing Instability in Intracycle Strain Hardening and Yield Stress Fluids to Create Roll-Coated Micro-scale Surfaces.” [draft available]
2. Perera, H., Khan, S., “Critical viscoelastic stresses in formation and shaping of melt spun hollow fibers.” [draft available]
3. Perera, H., Rahmanian, Khan, S., “Utilizing Physics Informed Machine Learning to understand dynamics of CO2 diffusion in Polystyrene.” [in preparation]
4. Perera, H., Khan, S., Hsiao, L. “Using high frequency rheology to measure fluid properties at high throughput.” [in preparation]
5. Islam, M. D., Perera, H., Black, B., Phillips, M., Chen, M.-J., Hodges, G., Jackman, A., Liu, Y., Kim, C.-J., Zikry, M., Khan, S., Zhu, Y., Pankow, M., Ryu, J. E., Template-Free Scalable Fabrication of Linearly Periodic Microstructures by Controlling Ribbing Defects Phenomenon in Forward Roll Coating for Multifunctional Applications. Adv. Mater. Interfaces 2022, 9, 2201237.

Skills

- Programming: Python, JAVA, C++, C, SQL
- Data science: Pandas, TensorFlow, DeepXDE, SciKit, OpenCV, SciKit
- Engineering Software: ANSYS, OpenFOAM, SOLIDWORKS, Arduino, Raspberry PI, Blender

Michael (Mike) J. Petrecca

Raleigh, NC 330-690-9690 mjpetrec@ncsu.edu www.linkedin.com/in/michael-petrecca

EDUCATION

North Carolina State University	Ph.D. Chemical and Biomolecular Engineering: 2019-2024	GPA: 3.79/4.00
The Ohio State University	BS Chemical Engineering, Minor in Economics: 2014-2019	GPA: 3.31/4.00

RESEARCH EXPERIENCE

North Carolina State University, Graduate Research Assistant. Advisors: Dr. Peter Fedkiw and Dr. Orlin Velev
Thesis Topic: Structural and electrochemical characterization of functional polymers for coatings and batteries
Project 1: Shear-derived dendritic redox polymer cathodes for Li-ion batteries
Project 2: Methods development for corrosion of powder-coated aluminum
Project 3: Shear-driven nanofabrication to produce polymer-based multi-functional components for Li-S batteries

The Ohio State University, Research Assistant in Dr. L.S. Fan's Clean Energy Lab (February 2017-May 2019)
- Assessed two-reactor and three-reactor system for hydrogen production from methane and ammonia using ASPEN PLUS simulations
- Designed and optimized separation scheme in CHEMCAD: 35% drop in energy requirements for ethylene recovery
- Managed all interviewing and onboarding of new undergraduate researchers into the lab

SKILLS AND PROFFICIENCIES

Laboratory/Analytical
- Electrochemistry: CV, EIS, GCD
- Li-ion and Li-S coin cell manufacture and testing
- Microscopy: optical, SEM, AFM
- Corrosion standards: DIN65472, ISO 4623, ASTM D2803, ASTM B117
- NMR, EPR, and FTIR
- Polymer synthesis and shear processing
- Glovebox operation and maintenance

Software
- Statistical design and analysis of experiments in JMP and MiniTab
- Electrochemical suites: Biologic EC Lab, Gamry EChem analyst
- Thermodynamic process simulation in ASPEN
- Image analysis in Fiji
- General experience in MATLAB and Python
- CAD design in SolidWorks

PUBLICATIONS

- Luiso, S.; **Petrecca, M.;** Williams, A.; Christopher, J.; Velev, O.D.; Pourdeyhimi, B.; Fedkiw, P.S.; "Structure-Performance Relationships of Li-ion Battery Separators" *ACS Appl. Polym. Mater.* 5, 3676-3686 (2022)
- Luiso, S.; Williams, A.H.; **Petrecca, M.J.**; Roh, S. Velev, O.D.; Fedkiw, P.S. "Poly(Vinylidene Difluoride) Soft Dendritic Colloids as Li-ion Battery Separators" *Journal of the Electrochemical Society* 168, 020517

SELECTED PRESENTATIONS

- **Petrecca, M.J.;** Shenoy, A.; Leatherman, J.R.; Velev, O.D.; Fedkiw, P.S.; "Next generation battery components derived from soft dendritic colloids" *244th ECS Meeting*, October 2023, Gothenburg, Sweden (Oral)
- **Petrecca, M.J.;** Kotb, Y.; Prout, J.; Basu, A.; Velev, O.D., Fedkiw, P.S.; "Filiform Corrosion on Polyester Powder-Coated Aluminum" *244th ECS Meeting*, October 2023, Gothenburg, Sweden (Poster)
- **Petrecca, M.J. ;**Shenoy, A.; Leatherman, J.R.; Velev, O.D.; Fedkiw, P.S.; "Shear-precipitation derived, nano-structured battery separators for next-generation energy storage" *97th ACS Colloids and Surface Science Symposium*, June 2023, Raleigh, NC. (Oral)
- **Petrecca, M.J.;** Christopher, J.; Velev, O.D.; Fedkiw. P.S.; "Applications of Soft Dendritic Colloids in Li-ion Batteries with Advanced Structure-Derived Performance" *242nd ECS Meeting,* October 2022, Atlanta, GA. (Poster)
- **Petrecca, M.J.;** Applications of Multifunctional Dendritic Polymers in Li-ion Batteries. *13th Beyond Li-ion Conference.* Virtually held at Argonne National Laboratory. June 2021. (Poster)
- **Petrecca, M.J.**; Clelland, K.; Christensen, T.; Kathe, M.; Fan, L.S.; Process Systems Simulations for Converting Ammonia to Hydrogen Using Chemical Looping. *2018 AIChE National Student Conference Poster Competition.* Pittsburg, PA. October 2018 (Poster)

INDUSTRY EXPERIENCE

Nexceris LLC, Development Intern (January-December 2018)
- Identified and resolved critical solid oxide fuel cell stack design constraints enabling 5 kW stack operation
- Designed, fabricated, and validated auto-thermal reformer-fed solid oxide fuel cell system for UAV application
- Troubleshot catalyst processing roadblocks by implementing standardized data collection form for variable tracking
- Implemented database connecting manufacturing specifications to R&D testing results for electrode formulations
- Became subject matter expert in gas delivery control stand design due to success in project execution

Schreiber Foods, Quality Assurance Intern (May -August 2017)
- Identified and controlled process variables impacting yogurt viscosity resulting in annual savings of $350,000
- Operated plant wide experiments to statistically validate effects of process alterations
- Conducted multiple capability studies to identify deficiencies in manufacturing practices and specs
- Sharpened project management skills with Six Sigma principles in creation of project charters

TEACHING EXPERIENCE

- NCSU, Fall 2021: CHE 713: Advanced Thermodynamics. Mentored Teaching Fellow
- NCSU, Summer 2021: CHE 543: Polymer Science and Technology. Graduate teaching assistant.
- NCSU, Spring 2021: CHE 715: Graduate Transport Phenomena. Graduate teaching assistant.
- NCSU, Fall 2020: CHE713: Advanced Thermodynamics. Graduate teaching assistant.
- OSU, Spring 2020: CBE 4760: Process Design and Economics. Undergraduate teaching assistant

AWARDS

- Mentored Teaching Fellowship for CHE 713 Aug 2021
- Student poster competition winner at 13th Beyond Li-ion Conference June 2021
- Ohio State Chemical Engineering Outstanding Undergraduate Award for Research Excellence April 2019
- 1st place in Fuels, Petrochemicals, and Energy division at AIChE Oct 2018
- 3rd place recipient of Harry West award for outstanding research in fuels and petrochemicals at AIChE Oct 2

LEADERSHIP EXPERIENCE

Fedkiw Research Group at North Carolina State University (Jan 2020 – Present)

Lab and Safety Manager (July 2020 – Present): Responsible for safe operation of research related activities
- Ensured safe and effective restart of research group, growing from 1 to 10 members over 3 years
- Mentored 12 undergraduate, 3 M.S., and 2 Ph.D. researchers spanning multiple projects

Triangle Electrochemical Society (Jan 2022 – Aug 2023)

Treasurer (Jan 2022 – Aug 2023): Responsible for managing budget of tri-university student organization
- Organized and secured sponsorships for summer student seminar series with NCSU, UNC, and Duke University.

North Carolina State University CBE Student Advisory Council (Sep 2021 – May 2022)
- Served on a student-led team focused on departmental enhancement through implementation of an anonymous reporting program, remodel of student lounge, and coordination of end of the year celebration

North Carolina State University CBE Graduate Student Recruiting (Jan 21 – May 21 & Jan 22 – May 22)

Head Graduate Recruiting Captain (’22 season): Team lead of 8 graduate student recruiting captains
- Team Lead: Planned, delegated, and ensured execution of first in-person recruiting weekends post-pandemic for 40 accepted students
- Team Member: (’21 season): Coordinated logistics of virtual meetings with faculty and current students

North Carolina State University CBE Graduate Student Association (Feb 2020 – July 2021)

President (July 2020 – July 2021): Ensured execution of all events to service graduate department
- Increased graduate student representation on executive board by 75% by implementing committees
- Led formation of interdepartmental mentoring program to connect early and senior graduate students
- Organized programming to maintain departmental engagement community within university pandemic guidelines

Treasurer (February – July 2020): Maintained budget and executed all purchasing for graduate department.

Jonathan D. Prout

Raleigh, NC, 27606 | jprout@ncsu.edu | 251-593-5052

Education

North Carolina State University - Raleigh, NC *Jan. 2022 - Dec. 2023*
Master of Science, Chemical and Biomolecular Engineering, GPA: 3.3/4.0
- Focus – Electrochemistry, Corrosion, Batteries

The University of Alabama, Tuscaloosa, AL, *Aug. 2014 - May 2017*
Bachelor of Science, Chemical and Biological Engineering, GPA: 3.0/4.0

Alabama Southern Community College - Monroeville, AL, *May 2013 - Aug. 2014*
- General Studies

Relevant Coursework/Research *Jan. 2022-Present*

Coursework: Electrochemistry, Polymer Science and Technology, Materials for Electrochemical Storage
Research: Electrochemical Corrosion of Organic Coatings, Peter Fedkiw Lab Group (NCSU)
- Studied corrosion of coated metals using electrochemical and optical techniques.
- Evaluated ability of corrosion resistance using coating structure property relationships of coatings.
- Planned and executed design of experiments to develop new methods for evaluating corrosion.
- Constructed cells for testing corrosion and developed standard operating procedures.

Work Experience

Mickey Leland Energy Fellowship - U.S. Department of Energy, Albany, OR *Jun. 2023 - Aug. 2023*
- **Research Associate**
  - Participated in research at the National Energy Technology Laboratory working with the Structural Materials team on coatings for natural gas pipelines protection.
  - Characterized surface of corrosion materials with SEM and EDS.
  - Evaluated response with electrochemical techniques with simulated hydrodynamic effects on corrosion.

Pratt Industries, Wapakoneta, OH
- **Stock Prep Process Engineer** *Oct. 2020 – Dec. 2021*
  - Worked with maintenance personnel to plan preventative maintenance improvements to save on costs by minimizing wear and tear on parts of equipment and piping.
  - Trained operators and helped develop protocols for operational standards of Stock Prep.
  - Improved operating safety of Paper Machine conditions with floor coating.
  - Assisted management of Capital Project worth $350K to improve maintenance costs and housekeeping efficiency.
  - Implemented process control logic by working with control engineers to improve automation of the process through the DCS system.
  - Collaborated and evaluated vendors to allocate proper resources, and plan out future uses of equipment and repairs.
  - Communicated with operations at the mill to changes in the process design and how to manage them.
  - Worked on process improvement projects to the operating mill.
  - Conducted mass balances and audited system to find points to improve efficiency of raw materials and saved on fiber loss by 5%.
  - Performed Start Up and Shutdown of new equipment to ensure its functional capabilities.
  - Learned and operated DCS control logic to improve the automation in the mill.
  - Assisted the transition of the mill from construction, commissioning, and production phases.
- **Project Engineer** *Dec. 2017 – Oct. 2019*
  - Assisted the project team working towards building a new start-up recycled linerboard paper mill worth up to $330M. Managed various projects under supervision worth up to $3M.
  - Managed installation of Paper Machine Hood and Air System from Scope of Installation to completion of project.
  - Managed purchase and installation of Floor and Tank coating of the entire mill.
  - Coordinated the purchasing and logistics of installing Cooling Towers.
  - Managed and tracked schedules of Contractors for chief project engineers.
  - Performed quality checks of contractors to ensure quality and track milestones for payments.
  - Assisted maintenance in Pump and belt alignments

Summer Discovery, Los Angeles, CA *Jun. 2017 - Aug. 2017*

- **Residential Counselor Internship** – Counselor on UCLA campus to high school students as they attended UCLA for the Summer discovery program and took classes. This helped me learn to work with people from different backgrounds as a team to help guide younger teens through this program.

The University of Alabama, University Medical Center, Tuscaloosa, AL *Sep. 2016 - May 2017*

- **Medical Scribe** – Assisted physicians in recording information during patient visits into the specialized medical computer system. Keeping confidentiality between patient and medical professional.

Alabama Southern Community College, Monroeville, AL Aug. 2013 – Jul. 2014

- **Math Tutor** – Met with students to help them learn and improve in mathematics classes. Learned best teaching practices for conveying concepts to different minded people.

Skills

- SEM and EDS techniques for surface characterization of materials
- Electrochemical techniques: PDP, EIS, LPR.
- Capital Project management for large scale projects/equipment.
- Data Processing using Potentiostat software, Excel, and Origin.
- Knowledge of piping and structural foundation installation methods.
- Worked with Distillation, CSTR, and Heat Exchanger units, as well as an Enzyme lab at Unit Operations Laboratory Experience, The University of Alabama, Summer 2016
- Computer languages – Microsoft Outlook, Word, Excel, PowerPoint, AutoCAD, Navisworks, MATLAB, Mathematica, ChemCAD, Polymath.

Leadership/Honors/Activities

- Eagle Scout – led Scouts in design, cost analysis, and implementation of Eagle project
- Interned with multiple types of doctors, shadowing them and learning about their career field. Viewed multiple surgeries to learn the details of these types of procedures.

Certificates:

- Boiler Operations Trained – CSD-1 under NFPA 85, knowledgeable and competent in boiler operations and design
- SAChE Chemical Process Safety
- SAChE Inherently Safer Design

Prottasha Sarker

625 Centennial Parkway, Apt 104, Raleigh, 27606 Tel: (336)-661-7754
Email: prottasha140@gmail.com | LinkedIn: prottasha-sarker-94a535147

EDUCATION

North Carolina State University — Raleigh, North Carolina
Doctor of Philosophy in Chemical and Biomolecular Engineering; GPA: 3.93/4.0 — *Aug 2019-Expected Graduation Jul 2024*

North Carolina State University — Raleigh, North Carolina
Master of Science in Chemical and Biomolecular Engineering; GPA: 3.93/4.0 — *Aug 2019-Dec 2021*

Bangladesh University of Engineering and Technology — Dhaka, Bangladesh
Bachelor of Science in Chemical Engineering; GPA: 3.92/4.0 — *Jul 2014 - Oct 2018*

AREA OF EXPERTISE

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

EXPERIENCE AND NOTABLE CONTRIBUTIONS

North Carolina State University — Raleigh, NC
Graduate Research Assistant — *Aug 2019 - Present*

- Advisor: Dr. Saad A. Khan and Dr. Orlando J. Rojas
- Research focus: Understanding the underlying interactions between the biomaterials involved and how they effect the bulk rheological properties
- The overarching goals of the current projects are:
  - Inquire how the injectability of pre-gel solution, gelation kinetics, final gel stiffness and yielding behavior of the collagen-based hydrogels get altered by introducing plant based tannic acid particles through rheological studies.
  - Explore the role of biodegradable morphology-controlled tannic acid particles on improving the mechanical properties of bio-based hydrogels for tissue regeneration applications.
  - Investigate the viability and metabolism of cells after the incorporation of tannic acid particles into collagen hydrogels.
  - Utilize isothermal titration calorimetry (ITC) technique to investigate the nature and extent of interaction between the biomaterials at different conditions.
  - Probe the underlying hydration and binding properties of collagen and morphology controlled tannic acid particles by varying pH conditions via quartz crystal microbalance (QCM).
  - Examine how difference in interacting behavior plays a role in regulating the final bulk properties of collagen-tannic acid particles composite.
  - Study how chitin nanocrystals interacts with different types of surfactants using isothermal titration caloriemetry (ITC).

North Carolina State University — Raleigh, NC
Graduate Teaching Assistant — *Aug 2020 - Dec 2022*

- Served as a TA for CHE 311H, Transport Processes I Honors (Fall 2020, Fall 2022), CHE 715, Fundamentals of Transport Phenomena (Spring 2021, Summer 2021)
- 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 — Dhaka, Bangladesh
Undergraduate Researcher — *Mar 2016 - Oct 2018*

- 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:
  - 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

- Danielle M. Nalband, Prottasha Sarker, Saad A. Khan and Donald O. Freytes, 'Characterization and Biological Evaluation of a Novel Flavonoid-Collagen Antioxidant Hydrogel with Cytoprotective Properties', Journal of Biomedical Materials Research: Part B - Applied Biomaterials, 2023
- Prottasha Sarker, Pallav K. Jani, Orlando J. Rojas and Saad A. Khan, 'Interacting Collagen and Tannic Acid particles: Uncovering pH-dependent Rheological and Thermodynamic Behaviors', Journal of Colloid and Interface Science, vol 650, part A, pp. 541-552, Nov 2023
- 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, vol. 23, no. 11, pp. 4696–4708, Nov 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, Aniqa 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

- "Understanding the interaction between pH responsive Collagen and Tannic Acid particles via Rheology and Thermodynamics", 97th ACS Colloids and Surface Science Symposium at Raleigh, North Carolina, June 04-07, 2023, 'Oral'
- "Rheology of collagen-based hydrogels tailored by tannic acid particles", Fall Schoenborn Graduate Research Symposium, NC State, October 31,2022, 'Poster'
- "Tuning the Rheology of Collagen-based Hydrogels using Tannic Acid Particles", 93rd Annual Meeting of The Society of Rheology at Chicago, Illinois, October 9-13,2022, 'Oral'
- "Rheology of collagen-based hydrogels tailored by tannic acid particles", 96th ACS Colloids and Surface Science Symposium at Golden, Colorado, July 10-13, 2022, 'Oral'
- "Modulating the Rheology of Collagen-based Hydrogels using Tannic acid Particles", Triangle Soft Matter Workshop, Duke University, May 9,2022, 'Poster'
- "Modulating the Rheology of Collagen-based Hydrogels using Morphology-controlled Tannic acid Particles" Fall Schoenborn Graduate Research Symposium, NC State, September 28,2021, 'Poster'
- "Modulating the rheology of collagen-based hydrogels using morphology-controlled tannic acid particles", 92nd Annual SoR Meeting, Bangor, Maine, October 10-14,2021, 'Poster'
- Annual Paper Meet- 2017, Chemical Engineering Division, The Institute of Engineers, Ramna, Dhaka-1000, Bangladesh, Oct 2017
- "Zero Discharge Effluent Treatment Plant", Fifth International Conference on Chemical Engineering: ICChE, Dhaka, Bangladesh, Dec 2017, 'Poster'

AWARDS & ACHIEVEMENTS

- 1st prize winner in CBE Research Image Contest, Chemical and Biomolecular Engineering Department, NC State, Spring 2023
- 3rd prize winner in Poster Competition, 2021 Fall Schoenborn Graduate Research Symposium, NC State, September 28,2021
- Provost Doctoral Fellowship, Fall 2019 through Fall 2020, North Carolina State University
- 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
- 1st prize winner in Poster Competition, Department of Chemical Engineering BUET, June 2016

SHERAFGHAN **IFTIKHAR**

RALEIGH, NORTH CAROLINA 27606 | 9194577524 | siftikh@ncsu.edu

Education

Ph.D.: **Chemical Engineering** — **08/2019-Present**
North Carolina. State University — Raleigh, NC, USA

Master of Science: **Chemical Engineering** — **07/2019**
University of Engineering and Technology — Lahore, Pakistan

Bachelor of Science: **Chemical Engineering** — **02/2014**
COMSATS University — Lahore, Pakistan

Experience

Graduate Teaching Assistance — **08/2019 to Present**
NC State University — **Raleigh, USA**

- Assist the faculty in teaching courses and developing teaching materials.
- Helping students with their assignments.

Graduate Teaching Assistance — **02/2018 to 02/2019**
University of Engineering and Technology — **Lahore, Pakistan**

- Assist the faculty in teaching lower-level courses and developing teaching materials.
- Assist the final-year students in their projects.
- Working with undergraduate students in the lab to help them conduct experiments.

Research Fellow — **12/2015 to 01/2017**
Pakistan Institute of Engineering and Appl. Sci. — **Islamabad, Pakistan**

- Topic: Study of Evaporation dynamics of Liquid Fuels, **Verification of D-Square Law**.
- Worked in the "Hazardous Air Pollutants Characterization and Control Laboratory".
- Prepared and maintained laboratory equipment prior to and after work.

Publications (Total Citations: 75)

1) $LaNi_xFe_{1-x}O_{3-\delta}$ as a Robust Redox Catalyst for CO_2 Splitting and Methane Partial Oxidation.
S Iftikhar, Q Jiang, Y Gao, J Liu, H Gu, L Neal, F Li; Energy & Fuels, **2021**

2) $LaNi_xFe_{1-x}O_3$ as flexible oxygen or carbon carriers for tunable syngas production and CO_2 utilization.
S Iftikhar, W Martin, Y Gao, X Yu, I Wang, Z Wu, F Li; Catalysis Today, **2022**

3) Ru-promoted perovskites as effective redox catalysts for CO_2 splitting and methane partial oxidation in a cyclic redox scheme.
S Iftikhar, W Martin, X Wang, J Liu, Y Gao, F Li; Nanoscale, **2022**

4) Comparison among various configurations of hybrid distillation-membrane setups for the energy efficiency improvement of bioethanol distillery: A simulation study.
S Iftikhar, Z Aslam, U Ali, A Akhtar; Journal of Chemical Technology & Biotechnology, **2021**

5) Final Technical Report for Sustainable Conversion of Carbon Dioxide and Shale Gas to Green Acetic Acid via a Thermochemical Cyclic Redox Scheme.
F Li, ***S Iftikhar***, L Neal North Carolina State Univ., Raleigh, NC (United States)

5) High-throughput oxygen chemical potential engineering of perovskite oxides for chemical looping applications.
X Wang, Y Gao, E Krzystowczyk, ***S Iftikhar***, J Dou, R Cai, H Wang, C Ruan, F Li; Energy & Env. Science, **2022**

6) Ce stabilized Ni–SrO as a catalytic phase transition sorbent for integrated CO_2 capture and CH_4 reforming.
H Gu, Y Gao, ***S Iftikhar***, F Li; Journal of Materials Chemistry, **2022**

7) Liquid Metal Shell as an Effective Iron Oxide Modifier for Redox-Based Hydrogen Production at Intermediate Temperatures.
X Wang, Y Gao, X Wang, R Cai, C Chung, ***S Iftikhar***, W Wang, F Li: ACS Catalysis; **2021**

8) Mechanically Robust, Thermally Insulating and Photo-Responsive Aerogels Designed from Sol-Gel Electrospun PVP-TiO2 Nanofibers**.**
V Rahmanian, T Pirzada, E Barbieri, ***S Iftikhar***, F Li, and S. A. Khan: Ap. Mat.Today; **2023 (Just Accepted)**

Conference Presentations

1) Ru-promoted perovskites for CO2-splitting and syngas generation in a Chemical Looping scheme.
S Iftikhar, W Martin, J Liu, Y Gao, I Wang and F Li; **2023** North American Catalysis Society Meeting.

2) Mixed Oxides As Flexible Carbon/Oxygen Carriers for Tunable Syngas Generation and CO_2 Utilization Under a Cyclic Scheme.
S Iftikhar, W Martin, X Wang, J Liu, Y Gao, and F Li; **2022** North American Catalysis Society Meeting.

3) Chemical Looping CO_2 splitting and Methane Reforming for Low-Carbon-Footprint Chemical Synthesis.
L Neal, ***S Iftikhar***, F Li, Y Gao; **2021** AIChE Annual Meeting.

Projects

1) Sustainable Conversion of Carbon Dioxide and Shale Gas to Green Acetic Acid via a Thermochemical Cyclic Redox Scheme. NC State University; **2019-2022**

   - **Role:** Picked Up the project in 2019 and took the lead. While working with my colleagues on this project, we produced some exciting data which we believe would be a significant contribution to the scientific community, especially to those areas targeting sustainable CO_2 utilization.
   - **Key Findings:** The key findings of this project were the development of redox materials capable of partially oxidizing methane and splitting CO_2 at low temperatures in a Hybrid Redox Process (HRP). The redox materials were not only efficient for HRP but also stable for long-term operations.
   - **Status:** Completed with all milestones met in a timely manner.

2) Microwave Catalysis for Process Intensified Modular Production of Carbon Nanomaterials from Natural Gas. NC State University; **2022-Present**

   - **Role:** Picked Up the project in 2022 and took the lead. This project mainly focuses on the production of clean COx-free hydrogen and Carbon Nanomaterials.
   - **Key Findings:** The key findings of this project so far include the efficient catalyst systems capable of thermally cracking methane at low temperatures. Our team at NC State is also working on other aspects such as process conditions and materials optimization for better hydrogen/carbon yield at low temperatures.
   - **Status:** This project is in progress and the milestones are being met in a timely manner.

Awards and Scholarships

1) **Vivian T. Stannett Graduate Award:** Vivian T. Stannett Graduate Award for Outstanding Early Publication recognizes research excellence, initiative, focus, and tenacity during the early career of Ph.D. students.
2) **Kokes Travel Award:** Kokes travel award for the 28th Annual North American Catalysis Conference held in Providence, Rhode Island, June 2023.
3) **Ph.D. Scholarship:** From the US – Pak Knowledge Corridor from the government of Pakistan.

Reference: References available on request.

MARIAM SOHAIL

Department of Chemical & Biomolecular Engineering
North Carolina State University
Raleigh, NC | 984-238-5376
msohail2@ncsu.edu

EDUCATION

North Carolina State University – USA
PhD (Chemical Engineering) – August 2019-July 2024
GPA: 3.83 / 4.00
Master of Science (Chemical Engineering) – 2019-2021
GPA: 3.83 / 4.00
NED University of Engineering & Technology – Pakistan
Master in Engineering (Chemical Engineering) – 2015-2018
GPA: 3.47 / 4.00
Bachelor in Engineering (Chemical Engineering) – 2010-2014
GPA: 3.65 / 4.00

WORK AND RESEARCH EXPERIENCE

North Carolina State University, Dept. of Chemical and Biomolecular Engineering (CBE), NC, USA
Research advisor: Dr. Saad Khan
Currently working as research assistant in the Khan Lab at CBE Department at North Carolina State University as a recipient of the Fulbright PhD scholarship. Primary research interests include:

- Characterizing system behavior of colloidal dispersions of polymer particles through correlating fundamental system properties to bulk dispersion behavior.
- Understanding rheological properties of surfactant-free Pickering Emulsions stabilized by polymer colloidal particles.
- Development of biodegradable controlled release polymer matrixes for loading agriculture Active Ingredients for achieving environmentally benign crop protection.
- Understanding and quantifying interactions between loading matrixes and Actives for achieving variable Active release rates.

Pakistan Petroleum Limited (PPL), Karachi, Pakistan
Associate, July 2017-July 2019
Served in different non-core departments as part of cross-functional rotation for training.
Sui Asset, July 2018 – July 2019
Served as an Associate Chemical Engineer in Plant Section of Sui, premium gas field of Pakistan, with responsibilities including but not limited to the following:

- Conducting technical evaluations of procured items and services.
- Assisting in budget development and tracking.
- Maintaining list of critical plant spares.
- Compiling daily gas production values.
- Assisting in formulation of Invitation to Bid (ITB) documents.

Cross functional rotation in different departments across PPL Enterprise Risk Management (ERM), June 2017 – June 2018

- Assisted Enterprise Risk Management team in assessing enterprise level risks across the organization, maintaining annual risk register and assisted in developing functional risk profiles for Assets/Departments.
- Underwent training in the Plant section of Sui Asset, and assisted in compiling the Monthly Performance Report (MPR) of Sui Field.
- Supported Community Development team in the monitoring and execution of PPL's various on-going Corporate Social Responsibility (CSR) projects operational at different gas producing fields.

- Served as an active member in the Procurement department assisting in procurement of Electrical & Instrumentation supplies across different fields.

PUBLICATIONS

- M. Sohail, T. Pirzada, R. Guenther, E. Barbieri, T. L. Sit, S. Menegatti, N. Crook, C. H. Opperman, S. A. Khan, "Cellulose acetate stabilized Pickering emulsions: preparation, rheology and incorporation of agricultural active ingredients, **ACS Sustainable Chemistry & Engineering**, in - press (2023)
- M. Sohail[#], T. Pirzada[#], C. H. Opperman, S. A. Khan, "Recent Advances in Seed Coating Technologies: Transitioning Toward Sustainable Agriculture" , **Green Chemistry**, (2022), https://doi.org/10.1039/D2GC02389J, [#]co-first authors
- T. Pirzada[#], M. Sohail[#], A. Tripathi, B. Farias, R. Mathew, C. Li, C. H. Opperman, S. A. Khan, Towards Sustainable Crop Protection: Aqueous Dispersions of Biodegradable Particles with Tunable Release and Rainfastness, **Advanced Functional Materials**, (2022) https://doi.org/10.1002/adfm.202108046, [#]co-first authors
- S. A. Taqvi, M. Sohail, F. Uddin. Utilization of Ion- Exchange Technology for Boiler Feed Water Production Design and Testing. **Chemical Engineering**, (2016) 1, 26-35

PRESENTATIONS

- **M. Sohail**, T. Pirzada, R. Guenther, E. Barbieri, C. H. Opperman, S. A. Khan. Rheology and applications of cellulose acetate stabilized Pickering emulsions. Oral presentation in American Chemical Society Fall 2023 National Meeting, August 13-17, 2023, San Francisco, CA, USA
- **M. Sohail**, T. Pirzada, R. Guenther, E. Barbieri, C. H. Opperman, S. A. Khan. Synthesis, rheology and applications of cellulose acetate stabilized Pickering emulsions. Oral presentation in 97th ACS Colloid & Surface Science Symposium, June 4-7, 2023, Raleigh, NC, USA
- **M. Sohail**, R. Hussain, T. Pirzada, S. A. Khan. Rheology of Pickering Emulsions stabilized via cellulose-derived nanoparticles. Oral presentation in 93rd Annual Meeting of The Society of Rheology, October 9-13, 2022, Chicago, IL, USA
- **M. Sohail**, T. Pirzada, C. H. Opperman, S. A. Khan. Cellulose Ester Colloidal Dispersions as Rainfast Biodegradable Foliar Formulations for Targeted Agrochemical Delivery. Oral presentation in 96th ACS Colloid & Surface Science Symposium, July 10-13, 2022, Golden, CO, USA

ACADEMIC HONORS

- 3rd place in the CBE Research Image Contest 2023, CBE Department, NC State.
- Inside back journal cover, Green Chemistry, August 2022
- Back journal cover, Advanced Functional Materials, May 2022
- Honorable Mention, NC State Research Image Contest, August 25, 2021
- Recipient of the Fulbright PhD scholarship 2019.

SKILLS

- Rheological analysis (flow, frequency, amplitude sweeps, microstructure) of emulsions and physical gels on TA-DHR rheometer.
- Nanoparticle size and morphological characterization through microscopic and light scattering techniques.
- SEM, goniometry, confocal and optical microscopy.
- Proficient in the use of MS Office, MATLAB, Imagej and Origin Pro.

UNIVERSITY SERVICE

- Lab Procurement Incharge: Fall 2020 – Spring 2023
- Teaching assistant for Graduate Advanced Chemical Engineering Thermodynamics (Fall 2020) and Undergraduate Thermodynamics of Chemical & Phase Equilibria (Spring 2021)
- Mentored research of four undergraduate (2) and master's (2) students.

Mann Manohar Verlekar

mverlek@ncsu.edu ❖ (984) 944-3907 ❖ http://www.linkedin.com/in/mann-verlekar

EDUCATION

North Carolina State University (NC State), Raleigh **Aug. 2022 - Present**
M.S. Chemical Engineering, Concentration in Upstream Biomanufacturing
GPA: 3.76/4

Relevant Coursework: Advanced Biomanufacturing and Biocatalysis, Fermentation of Recombinant Microorganisms, Molecular Biology for Biomanufacturing, Cell Line Development.

Birla Institute of Technology and Science (BITS), Pilani **Aug. 2017- July 2021**
B.E. Chemical Engineering
GPA: 7.72/10

WORK EXPERIENCE

Process Engineering Intern |AstraZeneca (via Kelly Services) **Jun. 2023 – Aug. 2023**
- Executed controlled experiments to develop novel porous particles involving the formulation and spray drying of emulsion batches over varying concentrations, homogenizing pressures and operating temperatures to assess yield and quality attributes.
- Conducted comprehensive analytical assays, including moisture content, particle size distribution, emulsion particle size, and compressed bulk density analysis.
- Contributed key insights to data-driven decision-making, aiding selection of viable candidates for further development.

Graduate Trainee – Engineering Leadership Programme | UltraTech Cement Ltd. **Sep. 2021 – May 2022**
- Developed a multiple regression model for the statistical analysis and optimisation of alkali-sulfur ratio in the hot meal with correlation to the process and quality parameters.
- Supervised the overhaul of Line II Cooler by leading a team in the replacement of brick lining, casting and removal of material buildups, resulting in increased recuperation efficiency and performance meeting project deliverables.

Project Intern | Birla Carbon **Jan. 2021 - June 2021**
- Studied the trends induced in the rotary dryer output due to the change in its parameters by building a CFD model and undertaking a simulation-based approach using SolidWorks and Ansys FLUENT.
- Evaluated the possibility of freeze-drying as an alternative by comparing the theoretical energy consumption and economic considerations between both methodologies for the same drying rate.

RESEARCH PROJECTS

Graduate Research Assistant | Wei Group **Feb. 2023 - May 2023**
- Contributed to the development of a CRISPR-Cas12a Dx assay for AAV detection, testing and comparing multiple reaction buffers and Cas12a enzymes.
- Adhered to strict SOPs and quality standards, maintaining reproducible testing conditions and ensuring reliability of assay outcomes.

Effect of Process Mode on Protein and scFv Fragment Production in E. coli **Jan. 2023 - Feb 2023**
- Studied the effects of batch and fed-batch production on growth rates, total recombinant protein production, and antibody fragment concentration in E. coli strain BL21.
- Performed ELISA and SDS Page Analysis to quantify the scFv13R4 fragment concentration.
- Demonstrated the increased cell growth and protein/scFv antibody expression in fed-batch samples at post-induction time points due to controlled substrate addition maximizing yield.

Influence of IPTG induction on Protein Enzymatic Activity in E. coli -Pfu CelB **Nov. 2022 – Dec. 2022**
- Conducted β-Glucosidase activity assay and Bradford protein assay to determine the impact of IPTG induction timings on enzymatic activity and total protein concentration respectively.
- Analyzed OD readings to show that earlier induction yielded lower cell densities but increased enzymatic

production at final timepoint.

Impact of Carbon Substrate on the Growth Rate of Recombinant E. coli **Oct. 2022 – Nov. 2022**

- Performed spectrophotometric quantification of specific growth rate and determined the effect of the carbon substrates* on max specific growth rate using One-way ANOVA. *(Glucose, Trehalose, Glycerol, and Glutamate)*
- Compared substrate-growth data groups using multiple t-tests to show that glucose induces the highest specific growth rate with its ease of incorporation into the citric acid cycle via glycolysis.

Capstone Project: Modeling of Carbon Black production using Ansys Chemkin **Aug. 2019 – Dec. 2019**

- Modeled the CB production process in a premixed burner utilising a discrete sectional approach to correlate the relationship between the operating conditions (*equivalence ratio, residence time*) to combustor performance.
- Worked on and modified a reaction mechanism code comprising 267 species, 991 conventional gas phase and 1855 reactions describing combustion, particle nucleation and growth.

SKILLS

- **Computational -** Ansys Chemkin, Aspen Plus, SolidWorks, Origin, IBM SPSS, MATLAB, ANOVA
- **Bioprocessing skills -** Centrifugation, Homogenization, Fermentation, Cell Culture, Clarification, Quality control, cGMP processes, Spray Drying, Aseptic Technique, IPTG Induction.
- **Analytical skills** - SDS-PAGE, Bradford Assay, ELISA, Gel Electrophoresis, UV Spectroscopy, Karl Fischer titration for Moisture Analysis, Malvern Zetasizer, CBD Analysis, Laser Diffraction for PSD, Nanodrop.
- **Failure/Deviation Investigation**: Process and Cleaning Validation, Equipment qualification, Documentation and writing SOP, Determining the root cause of process deviation and failures.

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 & Biomolecular Engineering *(Biotechnology and Biomanufacturing)*
- GPA 3.56/4.0

M.S. Chemical Engineering — May 2021

Virginia Tech (VT) – Blacksburg, VA — May 2018
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

PROFESSIONAL EXPERIENCES

Gene Therapy Co-op, *Biogen, Cambridge MA* — 07.2022-12.2022
Gene Therapy Cell Line Technology and Protein Cell Line Development groups
Managers: Dr. Danny Kim, Dr. Hooman Hefzi
- Generated Cas12a mediated Knockout mammalian cells lines, CHO and HEK293
- Single Cell Cloning, Hamilton Liquid Handling Systems, High Throughput Clone Screening, Fed Batch Culturing, Mammalian Cell Culture

Graduate Research and Teaching Assistant, *NC State University* — 01.2019-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 and mentoring two undergraduate researchers conducting independent research
- Yeast Surface Display, Protein Engineering, Flow Cytometry, Molecular Biology, Experimental design and Troubleshooting
- Completed coursework in protein interactions, viral biotechnology, downstream processing, and bioreactor design

Undergraduate Research Assistant, *Virginia Tech* — 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

Biomedical Engineering Intern, *Carilion Roanoke Memorial Hospital* — 2017
Virginia Tech-Carilion Clinic, Mark Skelton and Dr. Jake Soccha
- Shadowed biomedical engineers and physicians in various hospital departments

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
- Conducted chlorine and chloramine testing on waters in Columbia, SC

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.

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.

Alison C. Waldman

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

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. **Oral Presentation**. San Diego, CA. 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

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

- 2023 Graduate Recruitment Captain, Lead Captain
- 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

International Volunteer 2018

- Hillel at Virginia Tech, January. Quito & Morochos, Ecuador
- VT Engage, May-June. Puerto Maldonado, Urubamba (Sacred Valley) & Cusco, Peru

Alpha Omega Epsilon Sorority, Virginia Tech 2015-2018

- Executive Board, Secretary 2017-2018 academic year

Society of Agricultural and Biological Engineers (ASABE), Virginia Tech 2016-2018

- Chapter Secretary, 2016-2018, Awarded best chapter in the Southeastern Region, 2016-2017

Center for the Enhancement of Engineering Diversity (CEED), Virginia Tech 2014-2018

- 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 — August 2018 – Present
PhD Candidate
Minor in Biotechnology
Cumulative GPA: 4.00/4.00
Master of Science in Chemical Engineering — Received Fall 2020

Bucknell University, Lewisburg, PA
Bachelor of Science in Engineering — Graduated May 2015
Major: Chemical Engineering, **Concentration:** Materials Science
Cumulative GPA: 3.77/4.00; Engineering GPA: 3.90/4.00
Dean's List all academic semesters

University of Queensland, St. Lucia, QLD, Australia — July, 2013 – November 2013
Study Abroad during first semester of Junior year

Professional Experience

PhD Candidate, **Kelly Hyperthermophiles Group** at **North Carolina State University**, Raleigh, NC — 2019 – Present

- Metabolic engineering of thermoacidophilic Archaeon *Sulfolobus acidocaldarius*
- Investigation chemolithoautotrophic growth in thermoacidophilic Order Sulfolobales by sulfur oxidation
- Use of bioinformatics tools for comparative genomic evaluations, phylogenetic inference, and taxonomic reclassification
- Leverage comparative growth evaluation and transcriptomics to assess phenotypic variations
- Operation of bioreactors on 2L to 20L scales for generation of biomass and protein
- Isolation of recombinant protein in *E. coli* using induced expression and FPLC purification
- Long-read sequencing using Oxford Nanopore Technologies for *de novo* genome assembly and RNA-Seq
- Functional annotation and metabolic reconstruction for metabolic modeling through flux balance analysis
- Maintain lab operations as Safety Officer, Hazardous Waste Manager, and Lab Purchasing Coordinator

R&D Engineering Intern, **Novozymes** through **Qualified Staffing**, Franklinton, NC — Summer 2021

- 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

Chemist Engineer I, **Merck Pharmaceuticals** through **ExecuPharm**, Rahway, NJ — 2017-2018

- 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

Process Engineer, **Avery Dennison,** Painesville, OH — 2015 – 2017

- 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

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 it's Impact on Growth in *Sulfolobus acidocaldarius*." *J. Phys. Chem. B.* **125**(20): 5243-5257.

Bing, R.G.†, D.J. Willard†, M.J.H. Manesh, T. Laemthong, J.R. Crosby, M.W.W. Adams, and R.M. Kelly (2023). "Complete Genome Sequences for Two Thermophilic Indigenous Bacteria Isolated from Wheat Straw: *Thermoclostrodium stercorarium* subsp. RKWS1 and *Thermoanaerobacter* sp. RKWS2." *Microb. Resource. Announce.* **12**(3): 1-4.

Bing, R.G.†, D.J. Willard†, M.J.H. Manesh, T. Laemthong, J.R. Crosby, M.W.W. Adams, and R.M. Kelly (2023). "Complete Genome Sequences for *Caldicellulosiruptor acetigenus* DSM7040, *Caldicellulosiruptor morganii* (RT8.B8) DSM 8990 and *Caldicellulosiruptor naganoensis* (NA10) DSM 8991." *Microb. Resource Announce.* **12**(3): 1-3.

Willard, D.J., R.G. Bing, M.J.H Manesh, and R.M. Kelly. "Complete Genome Sequence for *Sulfuracidifex metallicus* DSM 6482." *Microb. Resource Announce.* (in preparation).

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., A. Recalde, C. Brasen, J.A. Counts, P. Nussbaum, J. Bost, L. Schocke, L. Shen, D.J. Willard, T.E.F. Quax, E. Peeters, B. Siebers, S.V. Albers, and R.M. Kelly (2021). "The Biology and Biotechnology of Archaeal Extreme Thermoacidophiles." *FEMS Microbiol. Rev.* **45**(4): 1-60.

Laemthong, T., A.M. Lewis, J.R. Crosby, R.G. Bing, W.H. Schneider, D.J. Willard, J.A. Counts, and R.M. Kelly (2022). "Enzymes from Extremely Thermophilic Bacteria and Archaea: Current State and Future Prospects." In *Extremozymes and their industrial applications* (N.A. Arora, S. Agnihotri, and J. Mishra, eds.), Microorganisms for Sustainability, Elsevier, pp. 41-84.

Bing, R.G., M.J. Carey, T. Laemthong, D.J. Willard, J.R. Crosby, D.B. Sulis, J.P. Wang, M.W.W. Adams, and R.M. Kelly (2023). "Fermentative Conversion of Unpretreated Plant Biomass: A Thermophilic Threshold for Indigenous Microbial Growth." *Bioresource Technol.* **367**: 12875.

Cooper, C.R., A.M. Lewis, J.S. Notey, A. Mukherjee, D.J. Willard, P.H. Blum, and R.M. Kelly (2023). "Interplay between Transcriptional Regulators and VapBC Toxin-Antitoxin Loci During Thermal Stress Response in Extremely Thermoacidophilic Archaea." *Environ. Microbiol.* **25**: 1200-1215.

Lewis, A.M., D.J. Willard, M.J.H. Manesh, S. Sivabalasarma, S.V. Albers, and R.M. Kelly (2023). "Stay or Go: Sulfolobales Biofilm Dispersal is Dependent on a Bifunctional VapB Antitoxin" *mBio*. **14**(2): 1-16.

Bing, R.G., D.J. Willard, J.R. Crosby, M.W.W Adams, and R.M. Kelly (2023). "Whither the genus *Caldicellulosiruptor* and the order Thermoanaerobacterales: phylogeny, taxonomy, ecology, and phenotype." *Front. Microbiol.* **14**: 1-15.

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)

Undergraduate Student Resume Packet

Daisy Aguilar Aguilar

daguila@ncsu.edu | daisyaguilaraguilar03@gmail.com | linkedin.com/in/Daisy-Aguilar-Aguilar | 919-464-1446 | Raleigh, NC.

Education

North Carolina State University (NCSU) | Raleigh, NC.

- Major: Chemical Engineering, concentration in Biomolecular Engineering *Anticipated May 2024*
- Minor: Biotechnology

Johnston Community College (JCC) | Smithfield, NC.

- Associates in Engineering & Associates in Science *May 2021*

Work Experience

Summer Intern | Shattuck Labs | Durham, NC. *Jun 2023-Aug 2023*

- Collaborated with the downstream team to successfully transcript the DNA template with targeted gene mTIGIT-Fc-LIGHT for expression in mammalian cells.
- Collaborated in the purification process of the mRNA made to use it in the formulation of different LNPs.
- Collaborated in the formulation of 15 different lipid nanoparticles (LNPs) to serve as the vehicle for the delivery of purified RNA into cells with the analytical development team as well as the formulation development team.
- Collaborated in the testing process for each LNP created with encapsulated RNA containing the gene of interest.
- Supported the troubleshooting process for arising problems during the testing of the LNPs' efficiency.

Undergraduate Researcher | San Miguel Lab at NCSU | Raleigh, NC *Jan 2022-present*

- Help in the improvement of a guillotine device capable of hurting *C. elegans* nematode for studying purposes.
- Supported the study of chemotaxis assays to develop new techniques to automate the count of the nematode *C. elegans*' behavior against different chemicals.
- Collaborated in the development of a coding program in MATLAB that is able to count the total number of worms in a plate scanned as well as perform and process the data obtained from the program.

Inbound Associate | Amazon | Garner, NC. *Sept. 2020-Sept 2021*

- Collaborated with the team in charge to deliver containers to other associates to upload them into the system.
- Controlled and improved the functionality of the damaged or delocalized drives used to store the pods in the designated floor area.

Camp Counselor | Johnston Community College| Smithfield, NC. *June 2021-July 2021*

- Collaborated with the Johnston Community College to deliver summer camps for kids related to the STEM field.

Line Operator | House Autry Mills Inc. | Four Oaks, NC. *Aug. 2019-Sept 2020*

- Operated complex machinery line productions.
- Collaborated with other line operators to achieve extra production assigned tasks.

Honors & Awards

- Goodnight Scholarship recipient |Goodnight Scholars| NCSU *May 2021- present*
- NC State's Women of Color grant recipient | NCSU *March 2020-May-2021*

Leadership & Civic Engagement

- University Ambassador at NCSU *April 2022 – present*
- Member of the CBE Departmental Diversity, Equity, and Inclusion committee *Sept 2023- present*
- Goodnight Transfer Retreat Leader *May 2022- Aug 2022*

Skills

- Fluent in English and Spanish. Capable of learning and manage complex processes in both languages.

Hannah Faye Dickerson

hfdicker@ncsu.edu | (919) 225-1894

EDUCATION:

- **North Carolina State University | Raleigh, NC** **May 2024**
  B.S. Chemical Engineering
  Minor In Biomanufacturing, Minor In Biological Science
  GPA: 4.0 / 4.0

PROFESSIONAL EXPERIENCE:

Abolhasani Lab | Undergraduate Research Assistant | Raleigh, NC **August 2021 - Present**

- Explored the ability of the flexible time and temperature-to-distance transformation to accelerate the discovery, development, and manufacturing of nanocrystal material through a novel modular flow reactor library.
- Constructed robust computational scaffolding in *Python* & *Labview* for analyzing transient phenomena, allowing the prediction of steady state behavior from dynamic, stepwise experimentation.
- Composed more than one version of the *Process Intensification Through Data Rich Approach: Dynamic Exploration Of Continuous Flow Quantum Dot Parameter Space* manuscript, which will be submitted for publication in *Chemical Science* by the end of this month. (September 2023)

Novozymes | Process Engineering Intern | Franklinton, NC **Summer, 2022 & 2023**

- Optimized the CIP (Cleaning In Place) process for the ultrafiltration membrane system, resulting in 3700000 GAL Of Water, 17000 MIN Of Production Time, and $75,000 + saved annually.
- Tested for microstability throughout the recovery process by performing an original crystal violet assay, which was later quantified through photographic pixel intensity analysis with *Image J.*
- Programmed an *Excel* tool to characterize company resource consumption; the tool is now used globally, plant wide.
- Devised an experimental framework for exploring soy grit consumption, with the ultimate goal of relating residual soy grit to batch contamination and yield.

HONORS & AWARDS:

Grand Challenge Scholar **Fall 2021 - Present**

- Exploring the intersection of engineering, entrepreneurship, and social consciousness, specifically focusing on their individual contribution to the engineering grand challenge of providing access to clean water.
- Traveled to El Batay, Dominican Republic for an immersive week with *Service For Peace,* spent installing the first water harvest system in the surrounding community.

University Honors College **Spring 2020 - Present**

- Immersed myself in the program's transformative learning experience characterized by unique, interdisciplinary coursework, culminating in my final capstone project.

NCNGA Academic Excellence Scholarship Recipient **Fall 2023**
Touchstone Energy Scholarship Recipient **Fall 2023**
Carl Stutts & Tessa Lesley Engineering Scholarship Recipient **Fall 2023**
REU Funding **Summer 2023, Fall 2023, Spring 2024**

PRESENTATIONS:

Dickerson H, Delgado-Licona F, Abolhasani M, Multi-Stage Flow Chemistry For Accelerated Quantum Dot Synthesis. Poster Presentation: 2023 ACC Meeting of the Minds; 2023 Mar 24-26; Blacksburg, VA.

Dickerson H, Delgado-Licona F, Abolhasani M, Multi-Stage Flow Chemistry For Accelerated Quantum Dot Synthesis. Poster Presentation: 2023 Southern Regional AIChE Conference; 2023 Mar 3-5; Gainesville, FL.

Dickerson H, Delgado-Licona F, Abolhasani M, Multi-Stage Flow Chemistry For Accelerated Quantum Dot Synthesis. Poster Presentation: 2023 GCSP Annual Meeting; 2023 Feb 26-28; Tempe, AZ.

Dickerson H, Delgado-Licona F, Abolhasani M, Multi-Stage Flow Chemistry For Accelerated Quantum Dot Synthesis. Poster Presentation: 2022 AIChE Annual Student Conference; 2022 Nov 11-14; Phoenix, AZ.

Jenna R. Kolbe

jrroger5@ncsu.edu | (919) 624-5015

OBJECTIVE

Junior Chemical Engineering student looking for a Process Engineering internship position during Summer 2024. Experience in process development, including bacterial transformation, fermentation optimization, and protein purification.

EDUCATION

NC State University | Raleigh, North Carolina Expected: May 2025
Bachelor of Science (B.S.) Chemical Engineering – Minoring in Biomanufacturing & Biotechnology
GPA: 4.0
Goodnight Transfer Scholars Program

Wake Technical Community College | Raleigh, North Carolina May 2020
Associate of Science, Associate of Engineering
GPA: 3.8
President Stephen C. Scott Scholarship 2019-2020
GlaxoSmithKline Endowed Scholarship 2018-2019

RELEVANT SKILLS

- SDS-PAGE
- Gel Electrophoresis
- Aseptic Techniques
- 2L Bioreactors
- *E. Coli* Fermentation
- qPCR
- Affinity Chromatography
- BCA Assay

WORK EXPERIENCE

Undergraduate Research Assistant - Dr. Qingshan Wei Lab, Chemical and Biomolecular Engineering, NC State University 5/2023-present

- Assist PhD candidate with a new project in the lab, expressing LbCas12a proteins in *E. Coli*.
- Complete literature review to discover methods of completing typical processes in our laboratory.
- Develop protocols for each step of the process, from plasmid extraction to protein characterization, using past laboratory experiments and literature.
- Troubleshoot when specific steps are unsuccessful to find a solution to keep up the project momentum.
- Present research updates in a technical presentation to Dr. Wei and other Wei Group PhD candidates.
- Presented my research at NC State University's 2023 Summer Undergraduate Research Symposium.

Customer Service | Chick-fil-a 7/2017-4/2019 | **Aqua-Tots Raleigh** 9/2018-2/2020 | **Fresh Market** Spring/Summer 2020 | **Carolina Pediatric Dentistry** 7/2020-6/2022

- Followed FDA, OSHA, and HIPPA regulations to ensure safety of all customers, patients, and employees.
- Assisted customers or patients while maintaining cleanliness of all work areas.
- Utilized communication skills with team members to ensure that all duties were completed in a timely manner while customers or patients remained the priority.
- Successfully handled stressful situations in which a customer or patient was disappointed with their experience by finding a solution myself or involving a manager for more escalated situations.
- Scribed for doctors during exams up to legal standards.
- Managed roughly 700 incoming phone calls per day as well as additional outgoing calls on a team of three individuals. Assisted in surgical scheduling and communications between Wake Med hospital and pediatric offices.
- Utilized my knowledge and skills at Aqua-Tots and Carolina Pediatric Dentistry to train new employees.

Hrishikesh Ram

2004 Weehawken Place, Apex, NC 27523

hram@ncsu.edu
www.linkedin.com/in/hrishikeshram
https://github.com/hrishikeshram27

OBJECTIVE

Prepare for an academic research career, seeking graduate studies in the chemical sciences. Areas of interest include computational chemistry, chemical kinetics and reaction engineering, and polymer physics, with environmental, biological, and energy applications.

EDUCATION

North Carolina State University, Raleigh, NC **August 2021 – May 2025 (Expected)**

B.S. Chemical Engineering & Chemistry GPA: 4.0/4.0

Minor: Music, Piano Performance Concentration

Dean's List (Fall 2021, Spring 2022, Fall 2022, Spring 2022)

Relevant Coursework: Material & Energy Balances, Transport Phenomena I/II, Chemical Thermodynamics, Phase and Reaction Equilibrium Thermodynamics, Kinetics and Reactor Engineering, Organic Chemistry I/II, Biochemistry, Systematic Inorganic Chemistry, Advanced Synthesis I/II, Quantum Chemistry/Statistical Thermodynamics, Physical Organic Chemistry

RESEARCH EXPERIENCE

Undergraduate Researcher **May 2021 – Present**

Westmoreland Group, Chemical and Biomolecular Engineering, NC State University

- Ongoing grant-funded project with US EPA to develop reaction mechanisms for thermal decomposition and incineration of PFAS (PFOA, PFOS) and corresponding metal carboxylate/sulfonate salts ("forever chemicals")
  - P.R. Westmoreland, **H. Ram**, T.P. Sadej, C.C. Murphy, "Elementary Reactions for PFAS Destruction Chemistry," 39th International Symposium on Combustion, Vancouver, Canada, July 24-29, 2022, Poster 3P052.
  - P.R. Westmoreland, **H. Ram**, T.P. Sadej, C.C. Murphy, "Present Status and New Results for PFAS Destruction Chemistry," AIChE Annual Meeting, Phoenix, AZ, November 13-18, 2022, Paper 654g.
- Techniques: density functional theory/electronic structure methods, statistical mechanics, elementary reaction rate theories (traditional and variational transition state theory), kinetic modeling, GCxGC-ToFMS, TGA/DSC, etc.

Summer Undergraduate Research Fellow **May 2022 – August 2022**

Materials Science and Engineering Division, Material Measurement Laboratory, NIST

- Ongoing project using density functional theory and molecular dynamics to quantify interaction energies between zwitterionic polybetaines and NaCl salt ions in aqueous solution
- Adapted the primitive quasichemical theory of ion solvation to compute polyion free energies in aqueous solution
- Developed NIST-internal Python package, "dft_toolbox", to automate the computational workflow for calculating aqueous free energies using quantum chemistry and molecular simulation

Research Intern **February 2020 – February 2021**

Echekki Group, Mechanical and Aerospace Engineering, NC State University

- Conducted deep learning methods for combustion chemistry data processing under Dr. Tarek Echekki
- Developed and optimized unsupervised noise-to-noise convolutional autoencoder algorithms in Python to denoise/post-process large experimentally-measured image datasets describing mass fractions and temperatures of chemical species in turbulent piloted-jet non-premixed flames
- Achieved ~0.97-0.99 correlation coefficient between desired and denoised data when applied to testing datasets from direct-numerical-simulation (DNS) with added Gaussian noise

SKILLS

- **Computational Techniques:** Electronic Structure/Quantum Chemistry Methods, Neural Networks/Deep Learning
- **Experimental Techniques:** TGA/DSC (TA Instruments), GCxGC-ToFMS (LECO)
- **Programming languages:** Python, MATLAB, C++, Java
- **Software:** Gaussian/Gaussview, ANSYS/CHEMKIN, RMG/Arkane (rmg.mit.edu), MESMER

HONORS AND AWARDS

- Theresa Mooney Freeman Scholarship, NC State College of Engineering
- Miriam Bailey Gardner Scholarship, NC State Dept. of Music

Amelia Shea

Raleigh, North Carolina • (252) 382-3354 • alshea@ncsu.edu

EDUCATION

North Carolina State University | Raleigh, NC — Anticipated May 2025

- 3.64 GPA
- Major: Chemical Engineering with a Biomolecular concentration

Millbrook High School | Raleigh, NC — June 2020

- 4.54 GPA; *Summa Cum Laude* Graduate

EXPERIENCE

ExxonMobil – Beaumont Refinery — May 2023 – Aug 2023

Light Oils Process Engineer Intern

- Progressed a case for action to optimize a reactor temperature curve by installing necessary equipment to better monitor general feed shifts - projected credits of $16.4M from additional LCO margin uplift
- Completed necessary sulfiding calculations in preparation for a unit turnaround to determine the total DMDS volume needed to fully activate the catalyst beds
- Established a salt deposition basis for heat exchangers in order to propose a recommendation for a more effective water wash method - potential savings of $720K by extending heat transfer life

Sylvamo – Eastover Mill

Utilities Process Engineer Co-op — Jan 2023 – May 2023

- Organized and led a vendor audit to generate a best practice review of current vendor-supplied equipment
- Determined a solution to improve sludge press polymer performance during conditions of high alkalinity and developed a trial plan for implementation
- Worked to improve water treatment equipment reliability and accuracy by troubleshooting sensor pluggages

Fibers Process Engineer Co-op — Jan 2022 – Aug 2022

- Led and completed a biannual moisture meter calibration which improved reading accuracy by about 3%
- Developed and implemented a trial to reduce departmental steam usage through pulp machine temperature adjustments – projected credits of $180K/year
- Developed a solution for better pulp machine pH control through the installation of a control scheme to reduce chemical and steam usage – projected credits of $115K/year

ACTIVITIES AND INVOLVEMENT

NCSU Undergraduate Research (Oct. 2021 – Present) | **NCSU Chemical & Biomolecular Engineering Student Ambassador** (Sept. 2021 – Present) | **American Institute of Chemical Engineers** (Aug. 2021 – Present)

SKILLS AND CERTIFICATIONS

- Lean Six-Sigma White Belt certification
- Proficient in developing codes using Python and VBA software
- Proficient with data analytical tools such as Minitab, Excel MI-Assist, Excel Solver, PROII Modeling, Excel Genie, and SEEQ

Christine Stark

| (919) 333-1109 | christine.r.stark@gmail.com

Objective

To obtain a full-time R&D position within a pharmaceutical/medical-focused company

Education

North Carolina State University, Raleigh, NC Expected: May 2024
Bachelor of Science in Chemical Engineering
Concentration in Biomolecular Sciences
Minors in Biotechnology and Tissue Engineering

Work Experience

Research, *Undergraduate Research Assistant*, Chapel Hill, NC Aug 2023-Present

- Microfluidic device design and fabrication
- Shear stress experimentations to examine nuclear stretches/movements under physiologically similar conditions.

Research, *Undergraduate Research Assistant,* Madison, WI May 2023-Aug 2023

- Worked with a post-doctoral student on a project testing capsular polysaccharide promoter expression under various stressors, such as pathogens in mice.
- Focused on cellular extraction from fecal matter, droplet microfluidic device fabrication and utilization, DNA purification and quantification.

Research, *Undergraduate Research Assistant,* Abolhasani Labs, Raleigh, NC Oct. 2021-Present

- Working with a Ph.D. student on the manganese doping of quantum dots to increase the range of colors available for production, we will be publishing a paper in a scientific journal.
- Working with a Ph.D. student on the production of lead-free quantum dots to limit adverse effects on the environment, we will be publishing a paper in a scientific journal.
- Working on a project of room temperature production and manganese doping of nanoplatelets.
- All projects require a flow reactor in order to produce respective products through flow chemistry.

Engineering Career Fair*, Coordinator,* Dec. 2021-Present

- Worked on the publicity and inventory subteams where we communicated with companies and students in addition to organizing the career fair.

Activities

- AIChE NCSU ChemE Cube Chair (Nov. 2022-Present)
  - Organize and lead meetings
  - Problem-solving combined with product design and build.
  - Structured a business plan
- Member of the American Insititute of Chemical Engineers (Aug. 2020-Present)
  - Poster presentation at the Southern Regional AIChE conference at the University of Florida
  - Poster presentation at the National AIChE conference in Orlando, Florida
- Member of the International Society for Pharmaceutical Engineers (Aug. 2022-Present)
  - Attended the National ISPE conference in Las Vegas, Nevada
- Poster presentation at the Schoenborn Research Symposium

Katherine Traynelis

ketrayne@ncsu.edu
(865) 210-2993

Education

North Carolina State University, Raleigh, NC — Graduation: May 2024
B.S. Chemical and Biomolecular Engineering
Minors: Biotechnology, Biomanufacturing
GPA: 4.0/4.0

Professional Experience

***Undergraduate Researcher* – Keung Research Group and Rao Research Group, NCSU Raleigh, NC**
Jan 2022-present

- Utilized molecular biology cloning techniques to troubleshoot and generate large scale yeast libraries for the testing of p300 acetyltransferase residue specificity
- Updated other lab members of research goals and results through oral presentations
- Generated Python scripts to assist my graduate student mentor in the analysis of NGS data

---

Awards

2023 Barry Goldwater Scholar
2023 Astronaut Scholar
2023 Southern Regional AIChE Student Technical Presentation first place winner
2022 AIChE Donald F Othmer Second Year Academic Excellence Award
2023 GGA Retreat Poster Contest Winner
REU funds: Fall 2023, Summer 2023, Spring 2023, and Spring 2022
Genetics and Genomics Academy 2023 Summer Team Mini Grant

Skills

Gel Electrophoresis
E. *Coli* and Yeast Cell Culture
Fluorescence Activated Cell Sorting
Next Generation DNA Sequencing Analysis
Basic Python
Molecular Biology Cloning
Flow Cytometry
Presentation/Public Speaking
Excel VBA

Presentations

Traynelis K, Waldman A, Keung AJ, Rao BM. High throughput mapping of epigenetic enzyme activity. Gulf Coast Undergraduate Research Symposium; 2023 Oct 20-22; Houston, TX.

Traynelis K, Waldman A, Keung AJ, Rao BM. High throughput mapping of epigenetic enzyme activity. Poster presented at: 2023 Schoenborn Research Symposium; 2023 Oct 3; Raleigh, NC.

Traynelis K, Waldman A, Keung AJ, Rao BM. High throughput mapping of epigenetic enzyme activity. Poster presented at: 2023 NCSU Genetics and Genomics Academy Annual Retreat; 2023 Aug 25; Raleigh, NC.

Traynelis K, Waldman A, Keung AJ, Rao BM. Investigating the residue specificity of p300 in human histone peptides. 2023 Astronaut Scholar Technical Conference; 2023 Aug 16-19; Orlando, FL.

Traynelis K, Waldman A, Keung AJ, Rao BM. Investigating the residue specificity of p300 in human histone peptides. 2023 ACC Meeting of the Minds; 2023 Mar 24-26; Blacksburg, VA.

Traynelis K, Waldman A, Keung AJ, Rao BM. Investigating the residue specificity of p300 in human histone peptides. 2023 Southern Regional AIChE Conference; 2023 Mar 3-5; Gainesville, FL.

Traynelis K, Waldman A, Keung AJ, Rao BM. Investigating the residue specificity of p300 in human histone peptides. Poster presented at: 2022 AIChE Annual Student Conference; 2022 Nov 11-14; Phoenix, AZ.
