UNIVERSITY OF DELAWARE
ENGINEERING

DEPARTMENT OF CHEMICAL
AND BIOMOLECULAR ENGINEERING

DOCTORAL CANDIDATES & POSTDOCTORATES

Resume Booklet
(2022-2023)

150 ACADEMY STREET, COLBURN LAB, NEWARK DE 19716

Chemical & Biomolecular Engineering
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Newark, DE 19716-3110
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January 2023

Dear Friends and Guests:

On behalf of the faculty of the Department of Chemical & Biomolecular Engineering, I am pleased to introduce to you candidates for professional careers at the doctoral or post-doctoral level. Many of them will be available for employment within the next year.

Delaware is one of the leading producers of chemical engineering PhDs in the country, with approximately 250 current graduate students, postdocs, and researchers in the department. The excellence of our department is especially evident in the graduate program, which continues to be ranked as one of the top ten in the United States.

Our students and faculty are driving new research initiatives across the wide range of chemical engineering science and practice—from biomolecular engineering to energy production and sustainable chemistry. A hallmark of the department is its leadership of strong interdisciplinary programs, centers, and institutes that connect faculty, students, industry, and national labs, including the UD-NIST Center for Neutron Science (CNS), Delaware Energy Institute (DEI), Center for Catalytic Science and Technology (CCST), the Catalysis Center for Energy Innovation (CCEI), Center for Biomanufacturing Science and Technology (CBST), Center for Research in Soft matter and Polymers (CRiSP), Center for Hybrid, Active, and Responsive Materials (CHARM), Center for Plastics Innovation (CPI), and the National Institute for Innovation in Manufacturing Biopharmaceuticals (NIIMBL). To learn more about these initiatives, the Department, our faculty and their research, and each of the students presenting today, I invite you to visit our web site www.che.udel.edu.

The department takes great pride in the successes and accomplishments of our students, who regularly receive awards, fellowships, and other recognitions for their research and teaching. But it is in their subsequent careers that they really come into their own. We are grateful for your interest in their future as potential employers, and we are certain that they will contribute strongly to your organizations. Please feel free to share this compilation of resumes with others in your company.

The concept and format for the fourth-year research symposium originated with our graduate student organization, the Colburn Club. It is an exceptional time to celebrate the leadership and creativity they bring to our community of engineering educators, learners, and scholars.

Sincerely,

Millicent O. Sullivan
Alvin B. and Julie O. Stiles Professor and Department Chair

UNIVERSITY OF DELAWARE
ENGINEERING
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2022-2023 CANDIDATES RESUMES

Angyal, Nicholas
Badejo, Oluwadare
Becker, Matthew
Bhoyar, Soumitra
Cassel, Samantha
Chen, Tso-Hsuan
Chen, Yingjie
Ding, Chaoying
Gupta, Yagya
Hansen, Kentaro
Kuo, Mi Jen
Lu, Shizhao
Luo, Yuqing
Oliveira, Nicholas
Oliveira, Alexandra
Paul, Brian
Selvam, Esun
Srinavas, Sanjana
Tian, Huayu
Vance, Brandon
Venkatarama Reddy, Jayanth
Yang, Piaoping
Yu, Kewei
Zare, Mehdi
Zhou, Jiahua

Nikolas Angyal

13 Oakley Ct, Newark, DE 19711
(845) 891-6066 | nangyal@udel.edu

Education

University of Delaware, 2019-present
Ph.D. Candidate in Chemical and Biomolecular Engineering

- Overall GPA: 3.93/4.0

University of Rochester, 2015-2019
B.S. in Chemical Engineering, *summa cum laude*

- Overall GPA: 3.99/4.0

Research Experience

Graduate Research Assistant in Dr. Marat Orazov's Group, 2019-present
University of Delaware – Newark, DE

- Conducted research on valorization of plastic waste and production of alpha-hydroxy acids through chemical pathways
- Using a model molecule for polyethylene, developed a procedure for oxyfunctionalization of polymer chains, followed by chain scission to give small, value-added oxygenates such as diacids, monoacids, alpha-hydroxy acids, ketoacids, etc.
- Developed and optimized a procedure for the high-yield production of lactic acid from acetone using a tandem reaction system
- Assistant Lab Safety Manager, 2020-present

Eisenberg Research Intern in Dr. Wyatt Tenhaeff's Group, June-August 2018
University of Rochester – Rochester, NY

- Conducted research on UV-cured vinyl ether (VE) polymer electrolytes for use in solid-state Li-ion batteries
- Developed a small-scale production method for reliable and reproducible manufacturing of the VE thin film electrolyte
- Characterized a novel ethyl VE polymer electrolyte via electrochemical impedance spectroscopy, cyclic voltammetry, Li/Li^+ cycling, and full cell Li-ion battery cycling

Work Experience

Petroleum Spills Intern, June-August 2017
New York State Department of Environmental Conservation – New Paltz, NY

- Under the direction of a NYS licensed PE, reviewed site investigation reports, work plans and closure reports for petroleum spill sites
- Lead DEC official on numerous spills, managing them through the clean-up process
- Researched and compiled information on large enforcement cases involving repeat offenders with many active spills to help harmonize clean-up and legal efforts

Skills

- **Experimental**: Gas Chromatography (GC), Mass Spectrometry (MS), Nuclear Magnetic Resonance Spectroscopy (NMR), X-ray Powder Diffraction (XRD), IR Spectroscopy
- **Software**: MatLab, Python, Origin, LabView, Minitab, Mathematica, ChemDraw, MestReNova, Microsoft Office

Teaching Experience

Graduate Teaching Assistant
University of Delaware – Newark, DE

- Diffusive Transport Processes: Fall 2021, Fall 2022
- Kinetic Processes: Fall 2021

Undergraduate Teaching Assistant
University of Rochester – Rochester, NY

- Fluid Dynamics: Spring 2018
- Organic Chemistry: Fall 2016, Spring 2017, Fall 2017

Volunteer Work

University of Rochester Young Alumni Council, 2020-present
University of Rochester YAC, Philadelphia Chapter – Philadelphia, PA

- Organized and ran various annual events such as Welcome to City, Annual Day of Service, New Year Celebration, Dandelion Day Celebration, and others for recent University of Rochester alumni in the Philadelphia area

Volunteer Assistant Coach, 2015-2019
East Fishkill Soccer Club – East Fishkill, NY

- Assisted in the running of training sessions
- Assisted in set-up and take-down of soccer fields

Classroom Volunteer, 2016-2018
Rochester International Academy – Rochester, NY

- Visited the school on a weekly basis to assist elementary school teachers in the classroom

Selected Activities and Affiliations

American Institute of Chemical Engineers, 2015-present
Tau Beta Pi Engineering Honor Society, 2017-present
Phi Beta Kappa Honor Society, 2018-present
University of Rochester Men's Varsity Soccer Team, 2016-2019

Honors and Awards

Collins Chemical Engineering Fellowship, 2020
CoSIDA Division III Academic All-American of the Year in Men's Soccer, 2018
CoSIDA Division III Academic All-American in Men's Soccer, 2017 and 2018
NCAA Division III Men's Soccer Elite 90 Academic Recognition Award, 2018
University of Rochester Dean's List, 8/8 semesters

Oluwadare A. Badejo

CONTACT INFORMATION:

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Wilmington, Delaware 19810

Email: badejo@udel.edu ; ooa.badejo@gmail.com

Mobile: +1 (302)-772-8871

LinkedIn: oluwadare-badejo

RESEARCH INTEREST:

Supply-Chain Optimization (Integrated, Modular, Supply chain under disruption), Production Scheduling, Stochastic and Mixed integer programming , Process control & optimization, Machine learning, and Data science

EDUCATION:

University of Delaware, Newark DE — Aug. 2019 – Present
Ph.D. Candidate, Chemical and Biomolecular Engineering
Advisor: Prof. Marianthi Ierapetritou

University of Lagos, Lagos, Nigeria — Jan. 2011 – Dec 2015
Bachelor of Chemical Engineering

WORK EXPERIENCE:

University of Delaware, Department of Chemical and Biomolecular Engineering
Graduate Research Assistant — Aug. 2019 – Present

Developed stochastic optimization-based supply chain model for modular plants. This model proposed production plan that improved overall demand satisfaction under variety of scenarios (ranging from best case to worse case)

Designed Integrated supply chain model that captured three supply chain levels (scheduling, operational, and strategic levels) using MINLP model motivated by machine learning.

Developed a supply chain optimization model that facilitates decision-making during disruptions. The model captures optimal actions to ensure robustness during disruptions and simultaneously manage operational uncertainties.

University of Lagos, Department of Chemical and Petroleum Engineering
Graduate Research Assistant, — July 2018 – Aug. 2019

Combined teaching, research, administration, and management increased department production. Supervised four courses and built a mentorship structure, leading to exceptional results.

Eunisell Limited Lagos/Rivers State
Oilfield Engineer, — Jan. 2018 – June 2018

Technical Oilfield Chemicals. Improved methodology for offering process-engineering consultancy to oil and gas exploration businesses, increasing clientele base.

Spunt Innovatia Lagos
Technical Trainer , — April 2017 – Dec. 2017

Orchestrated a training and development system for university staffs and students on chemical engineering software (encouraging open source software) leading to higher productive levels for team.

Landmark University, Omu-Aran, Kwara State
Research Assistant, — April 2016 – March 2017

Research, teaching, and student management experience. aided in the development of experiments with the objective of increasing students' scientific literacy. Coordinated lectures and tutorials to improve student learning. Developed a feedback method for students' strengths and weaknesses, resulting in improved performance.

Shell Petroleum Development Company of Nigeria, Rivers state
Process Engineering Intern Aug. 2014 – Dec. 2014
Worked with the asset and optimization team to resolve the challenges of a non-associated gas plant using process simulation models validated with field data.
Communicated sophisticated simulation models to teams and management without engineering knowledge.

JOURNAL PUBLICATIONS :

Ierapetritou, M., **Badejo, O.,** 2022. A Mathematical Modeling approach for Supply Chain Management under Disruption and Operational Uncertainty. Authorea Preprints.

Badejo, O., Ierapetritou, M., 2022a. Mathematical Programming Approach to Optimize Tactical and Operational Supply Chain Decisions under Disruptions. Ind. Eng. Chem. Res. https://doi.org/10.1021/acs.iecr.2c01641

Badejo, O., Ierapetritou, M., 2022b. Integrating tactical planning, operational planning and scheduling using data-driven feasibility analysis. Computers & Chemical Engineering 161, 107759. https://doi.org/10.1016/j.compchemeng.2022.107759

Bhosekar, A., **Badejo, O.**, Ierapetritou, M., 2021. Modular supply chain optimization considering demand uncertainty to manage risk. AIChE Journal n/a, e17367. https://doi.org/10.1002/aic.17367

Babalola, F.U., **Badejo, O.A.**, Roy-Layinde, B.A., 2019. Emerging challenges in phase behavior modeling of reservoir fluids at high-pressure high-temperature (HPHT) conditions. Geomechanics and Geophysics for Geo-Energy and Geo-Resources 5, 357–370.

AWARD RECOGNITIONS:

First prize, 2016 NSChE annual design project contest, for the best design project
Best graduating student 2015 set, Department of Chemical Engineering, University of Lagos.

LEADERSHIP POSITION:

Public Relations Officer (volunteer position)
Drug Free Community Development Group April 2016 – March 2017
Acted as the public relations officer, Organized sensitization for community members & schools educating them about the effects of drugs

President/founding members
Academic Resource Team (University of Lagos) Jan. 2012 – Dec.2015
Organized the first design paper competition and championed the fund-raising campaign.

Electoral Committee's General Secretary *(*University of Lagos) July 2013
Organized a departmental election and served as a liaison between the Electoral Committee, the Office of Student Affairs, and the students.

COMPUTER SKILLS:

GAMS, Python, MATLAB, R, SQL, Microsoft Office Suit, LATEX

Matthew L. Becker

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Elkton, MD 21921

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✉ matt3@me.com
✉ beckerml@udel.edu

Education

- **The University of Delaware**, Newark, DE — August 2019 - Present
  PhD in Chemical and Biomolecular Engineering — GPA: 3.53/4.00
  Advisor: Prof. Abraham M. Lenhoff

- **The Pennsylvania State University**, University Park, PA — August 2014 - May 2018
  Dual-BS in Chemical Engineering and Economics — GPA: 3.81/4.00
  Thesis: Purification, Crystallization, and Analysis of Various OmpF Mutants and Their Block Copolymer Aggregates for Use in the Production of Biomimetic Membranes

Research Experience

- **Development of a Purification Process by Continuous Affinity Precipitation**
  Doctoral Research, The University of Delaware, Newark, DE — September 2021 – Present
  Principal Investigator: Prof. Abraham M. Lenhoff
  - Developing small-scale purification system with eye for eventual possible tech transfer
  - Studying kinetics of model system using zinc chloride chelator and mAb in batch and continuous mode
  - Implementing control system to facilitate removal of drastic system changes from minute perturbations

- **Characterization of the Binding Behavior of Host Cell Proteins to Monoclonal Antibodies**
  Doctoral Research, The University of Delaware, Newark, DE — January 2020 – September 2021
  Principal Investigator: Prof. Abraham M. Lenhoff
  - Investigated binding strength of HCPs to a library of industry mAbs
  - Identified binding residues on persistent HCPs and on mAbs in-library
  - Assisted with research that resulted in a crucial discovery of HCP-heavy aggregates persisting through various process steps

- **Investigation of OmpF Proteins as Part of Block Copolymers for Use in Biomimetic Membranes**
  Undergraduate Research, The Pennsylvania State University, University Park, PA May 2016 – May 2018
  Principal Investigator: Prof. Manish Kumar
  - Developed and performed optimal method to ensure pure and high-yield OmpF samples
  - Analyzed the microscopic appearance of different ratios of various mutants of OmpF to polymer

- **Analysis of Process Condition Effects on Bacterial Polysaccharides**
  Undergraduate Research, The Pennsylvania State University — May 2015 – May 2016
  Principal Investigator: Prof. Andrew L. Zydney

- Evaluated filtrate flux in TFF stirred cell for both model dextran solution and polysaccharide solution
- Conducted tests at various feed pressure conditions in order to determine optical conditions for flux over time while avoiding significant membrane fouling

Skills

- Proficient in fluorescence and absorbance spectroscopy, mass spectrometry, TFF, dialysis, and process design
- Programming in MATLAB, Mathematica, MINITAB, and scripting in BASH for data manipulation and automation.

Leadership and Recognition

- Chosen by fellow graduate students to be second year representative (2020) and co-president (2021) of Colburn Club for UD ChBE, organizing events and providing leadership
- Selected as EmPOWER mentor for UD ChBE in 2019, helping to mentor incoming first-year students
- Received top marks from students in 3/3 classes TA'ed as a graduate student
- PSUCOE Summer Research Participant and Excellence in Summer Research Award Winner (2015)

Selected Publications (* indicates co-first author; † indicates not yet submitted; ‡ indicates in preparation)

1. †Y. Oh*, M. L. Becker*, K. M. Mendola, L. H. Choe, K. H. Lee, Y. Yigzaw, A. Seay, J. Bill, X. Li, D. J. Roush, S. M. Cramer, S. Menegatti, A. M. Lenhoff. Factors Affecting Product Association as a Mechanism of Host-Cell Protein Persistence in Bioprocessing.
2. ‡M. L. Becker, X. Han, M. Vats, S. Parasnavis, Y. Yigzaw, A. Seay, J. Bill, X. Li, D. J. Roush, S. M. Cramer, S. Menegatti, A. M. Lenhoff. Experimental and Computational Analysis of Binding Site Residues in Host Cell Protein and Monoclonal Antibody Binding.

Selected Conference Proceedings

1. M. L. Becker, Y. Oh, K. M. Mendola, A. Seay, X. Li, D. J. Roush, S. M. Cramer, S. Menegatti, A. M. Lenhoff. Biophysical Characterization of Problematic Host Cell Proteins in Monoclonal Antibody Processing. *ACS BIOT*, August 2021.

Soumitra Bhoyar

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Google Scholar | LinkedIn

Education

- **The University of Delaware**, Newark, DE, USA — 2019 - *present*
  PhD student, Chemical and Biomolecular Engineering
  Advisor: Dr. Abraham M. Lenhoff
- **The Johns Hopkins University**, Baltimore, MD, USA — 2016 - 2018
  Masters in Chemical and Biomolecular Engineering
  Advisor: Dr. Daniele M. Gilkes
- **The Institute of Chemical Technology**, Mumbai, India — 2010 - 2014
  Bachelors in Chemical Engineering

Research Experience

- **The role of high-pH effects in antibody–protein A interactions** Doctoral Research, The University of Delaware — 2020 – *present*
  - Designed, expressed and purified a novel protein A ligand, tailored to mitigate monoclonal antibody yield loss under high-pH washes in protein A chromatography.
  - Identifying the mechanisms leading to dissociation of the IgG1–protein A complex at high pH.
- **Protein A chromatography modeling**
  Doctoral Research, The University of Delaware — 2019 – *present*
  - Developing a mechanistic, predictive model for protein A chromatography
- **Image analysis in breast cancer**
  Masters Thesis, The Johns Hopkins University — 2016 – 2018
  - Developed image-analysis based assays for a more quantitative understanding of breast cancer metastasis.
  - Determined the role of human beta-6-tubulin (TUBB6) on cancer proliferation and chemoresistance under hypoxic and normoxic conditions.

Work Experience

- **Indiahikes**
  Trek Leader — 2018 – 2019
  - Led high-altitude trekking teams in the Indian Himalayas, at altitudes of ∼16,000 feet.
  - Trained in identifying and resolving high altitude medical conditions such as pulmonary and cerebral edema.
- **Honeywell-UOP**
  Design Engineer — 2014 – 2016
  - Designed simulations and process equipment for commercial oil refineries
  - Mediated technical discussions involving customers, field specialists and project management.
  - Obtained the Six-Sigma Green Belt certification.

Publications

1. H. L. Rocha, I. Godet, F. Kurtoglu, J. Metzcar, K. Konstantinopoulos, S. Bhoyar, D. M. Gilkes, and P. Macklin. A persistent invasive phenotype in post-hypoxic tumor cells is revealed by fate mapping and computational modeling *iScience*, 24 (9), 2021.
2. S. Bhoyar, I. Godet, J. W. DiGiacomo, and D. M. Gilkes. A software tool for the quantification of metastatic colony growth dynamics and size distributions in vitro and in vivo *PloS one*, 13 (12), 2018.

Conference Proceedings

1. S. Bhoyar, X. Xu, S. Traylor, J. Guo, S. Ghose, and A. M. Lenhoff. Determinants of capacity of Fc-based antibody structures in protein A chromatography. *ACS BIOT*, Aug 22-26, 2021.
2. I. Godet, J. Ju, S. Bhoyar, G. Wang, S. Sukumar, and D. M. Gilkes. Hypoxia-reporter construct helps to uncover the metastatic process. *EACR Seed and Soil: In Vivo Models of Metastasis*, Nov 27-29, 2017.

Skills

- **Chromatography:** Proficient in the use of liquid chromatography systems, chromatographic columns and resins.
- **Biophysics:** Circular dichroism spectroscopy, dynamic light scattering, biolayer interferometry, HPLC, surface plasmon resonance, UV-vis spectrometry.
- **Cell culture:** Bacterial and mammalian cell culture, protein expression and purification, and genetic manipulations of bacterial cell lines.
- **Software and Programming:** CADET (Chromatography analysis and design toolkit), Python, MATLAB, Mathematica, and scripting in AWK and BASH for data manipulation and automation.

Leadership and Recognition

- Co-Leader of EmPOWER, the departmental peer-mentorship group at the University of Delaware, 2022.
- Co-Leader of Colburn Club, the ChemBE graduate student organization at the University of Delaware, 2021.
- Selected by the department to be to be the **Schipper fellow**, 2020.
- Awarded the **Bravo award** by Honeywell-UOP for excellence in technical work, 2016.

Samantha E. Cassel

PhD Candidate
Chemical and Biomolecular Engineering
University of Delaware, 590 Avenue 1743, Newark DE 19713

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EDUCATION

Ph.D. Candidate in Chemical Engineering Fall 2017 – present
University of Delaware, Newark DE *anticipated graduation: May 2023*

M.S. in Biomedical Engineering *Accelerated Dual Degree Program* 2017
Drexel University, Philadelphia PA

B.S. in Biomedical Engineering *Biomaterials and Tissue Engineering*, *Summa Cum Laude* 2017
Drexel University, Philadelphia PA

RESEARCH EXPERIENCE

Graduate Research Assistant *Advisor: Prof. April Kloxin* Fall 2017 – present
University of Delaware, Department of Chemical and Biomolecular Engineering

Development of a dynamic, lentiviral-based dual fluorescence reporter of fibroblast activation for investigation of fibrosis disease mechanisms in multidimensional culture systems

- Optimized lentiviral production for multiple fluorescent reporter systems and established robust transduction protocols for cell lines and primary cells
- Established 15+ stable cell lines for reporting temporal dynamics of alpha smooth muscle actin (aSMA) expression
- Developed confocal live-imaging and image-analysis protocols to track and quantify protein expression dynamics
- Developed statistical data-analysis methods for assessing heterogeneous fibroblast population distributions
- Encapsulated reporter cell lines and primary cells in hydrogel systems and assessed response (viability, migration, protein expression) to multiple stimuli (fibrillar structure, biochemical cues, co-culture interactions)
- Synthesized, purified, and characterized self-assembling, fibrillar peptides and functionalized polymer macromers for covalent incorporation (thiol-ene click chemistry) into 3D hydrogel cell culture platforms
- Characterized mechanical properties (formation, degradation, equilibrium) of hydrogel platforms by shear rheometry

RESEARCH SKILLS

Mammalian Culture/Assessment	Bacterial Culture	Materials Synthesis/Characterization	Computer
Lentivirus production	Transformation	Solid phase peptide synthesis	MS Office
Stable cell line production	Ligation	Polymer end-group modification	MATLAB
Flow cytometry/FACS	Plasmid purification	Shear rheometry	Python
Immunostaining	Gel electrophoresis	Click chemistry	Minitab
Confocal microscopy	Site-directed mutagenesis	Reverse-phase HPLC	ImageJ
3D hydrogel encapsulation		Mass spectroscopy (ESI, LC-MS)	Origin Labs
Viability/metabolic assays		Circular dichroism	Volocity
DNA/RNA isolation		UV-Vis spectroscopy	Imaris
RT-qPCR		^{1}H NMR	

PROFESSIONAL EXPERIENCE

Biomaterials R&D Engineering Co-op Fall 2015 – Spring 2016
DePuy Synthes, Bone Graft Substitutes, West Chester PA

- Conducted cross-linking, degradation, and mechanical testing on polymers and composites
- Developed rheological methods for characterizing stability of polymers to optimize storage conditions

Quality Engineering Co-op Fall 2014 – Spring 2015
Secant Medical, LLC, Quality Engineering, Perkasie PA

- Developed Failure Modes and Effects Analysis (FMEA) reports for textile production processes and presented results
- Designed and implemented Test Method Validation (TMV) protocols
- Analyzed datasets for Process & Operational Qualifications (PQ/POQ) of development products

PROFESSIONAL EXPERIENCE (cont.)

Clinical Research Assistant Fall 2013 – Spring 2014

Thomas Jefferson University, Department of Emergency Medicine, Philadelphia PA

- Conducted screening and informed consent in research subject recruitment
- Revised protocols and regulatory documents for submission to Institutional Review Board
- Collaborated with research coordinators to troubleshoot and revise recruitment methods

LEADERSHIP EXPERIENCE

Chemical and Biomolecular Engineering Representative, Women in Engineering Steering Committee 2020 – 2022

- Led the organization and execution of two college-wide events per semester
- Developed new programming to further the goal of advocacy and representation of women in engineering

Committee Lead & **Peer Mentor**, Empathetic Peers Offering Wisdom Encouragement, & Resources 2019 – 2022

- Mentored 2-3 incoming first year students each year to aid in their transition to graduate school
- Collaborated to develop and organize professional development events to assist students in all program years

President, Colburn Club (Chemical and Biomolecular Engineering graduate student organization) 2019 – 2020

- Collaborated with staff & faculty to organize two recruitment weekends for up to 40 visiting students, including one rapid pivot to a virtual recruitment experience in March 2020
- Managed team of 50-60 graduate student volunteers for successful execution of recruitment events
- Lead team of 10-12 graduate student leaders in planning professional development and social events for all department graduate students

TEACHING EXPERIENCE [number of students enrolled]

CHEG112: Introduction to Chemical Engineering [125], *University of Delaware* Spring 2019
CHEG332: Chemical Engineering Kinetics [74], *University of Delaware* Fall 2018
BMES505/506/507: Mathematics for the Biomedical Sciences I/II/III [31/28/22], *Drexel University* 2016-17
Math Tutor, Serviam Girls Academy (grades 5-8), New Castle DE 2017 – 2021

SELECTED PEER-REVIEWED PUBLICATIONS equal contribution*

1. **SE Cassel** and AM Kloxin. "Establishment of a dynamic reporter for assessing real-time activation of wound healing cells" **in preparation**, 2022
2. K Bomb*, PJ LeValley*, I Woodward, **SE Cassel**, et al. "Biomaterial and flow-based membrane technologies for improved biomanufacturing of T-cell therapies," *Advanced Materials Technologies*. **Accepted** November 2022
3. KA Wodzanowski*, **SE Cassel***, CL Grimes, and AM Kloxin. "Tools for probing host-bacteria interactions in the gut microenvironment: from molecular to cellular levels" *Bioorganic & Medicinal Chemistry Letters*, **30,** 127116, 2020. DOI: 10.1016/j.bmcl.2020.127116
4. ME Smithmyer, **SE Cassel**, and AM Kloxin. "Bridging 2D and 3D culture: probing impact of extracellular environment on fibroblast activation in layered hydrogels" *AIChE J*, Futures Issue, 2019.
5. ME Smithmyer, CC Deng, **SE Cassel**, PJ LeValley, BS Sumerlin, and AM Kloxin. "Self healing boronic acid-based hydrogels for 3D co-cultures" *ACS Macro Letters*, **7**, 1105-1110, 2018.

SELECTED CONFERENCE PRESENTATIONS

1. **SE Cassel** and AM Kloxin. "Lentiviral-based fluorescent reporters for assessing human lung fibroblast activation in response to microenvironmental stimuli." *Oral Presentation* at 2022 AIChE Annual Meeting
2. **SE Cassel** and AM Kloxin. "Lentiviral reporters for temporal characterization of cell activation in response to dynamic stimuli." *Oral Presentation* at 2022 Annual Society for Biomaterials Meeting; April 27-30; Baltimore, MD

HONORS & AWARDS

Saurabh A. Palkar Graduate Award for Mentoring Fellowship 2022
Robert L. Pigford Teaching Assistant Award 2020

Tso-Hsuan (Eric) Chen

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EDUCATION

University of Delaware **September 2018-Present**
Ph.D. Chemical Engineering
National Taiwan University **September 2013-June 2017**
B.S. Chemical Engineering

PROFESSIONAL EXPERIENCE

Vlachos' Lab, Ph.D. Student **September 2018-Present**

- Developed the mechanism and kinetics of the direct acylation reaction of furan over various catalysts using density functional theory (DFT) calculations and microkinetic modeling (MKM).
- Collaborated with the Tsapatsis' group to determine the most probable structure of the phosphate-modified UiO-66 MOF and understood the impact of NDS ligand substitution on the water stability of MOF-808 using DFT calculations.
- Revealed the unexpected solvent effect for fructose dehydration in biphasic systems using classical molecular dynamics (MD) and quantum mechanics/molecular mechanics (QM/MM) MD simulations and determined a powerful descriptor that could predict the selectivity under different solvents.
- Elucidated the effect of entropy, OH/Pd coverage, temperature, surface termination, metal/support dynamics and the role of Sn on the kinetics and thermodynamics of the nucleation of Pd_2, Pt_2 and Pt-Sn on the alumina support using ab initio MD (AIMD) in conjunction with thermodynamic integration (TI) and metadynamics (MTD) methods.
- Built neural network potentials (NNPs) for zeolites and explored the changes of translational and rotational entropies for substrates during reaction in confined environments.

Precise Printing Technology Lab, Research Assistant **July 2017-April 2018**

- Collaborated with the Taiwan Textile Research Institute to develop novel aerial filtration models for predicting the behavior of oil drop on non-woven fabrics using COMSOL simulations.
- Fabricated a hydrophobic but oleophilic foam that could be used for the oil-mist removal.

Precise Printing Technology Lab, Research Undergraduate **February 2016-June 2017**

- Fabricated stretchable 3D conductive patterns using Inkjet printing.
- Developed healable and conductive patterns on foldable and extremely rough substrates.
- Designed an integrated sensor for temperature and humidity tracking by Inkjet printing.

Asmedia Technology Inc., Internship **June 2015-September 2015**

- Designed and improved integrated circuits (IC).
- Tracked the quality of chip manufacturing.

SKILLS

Expertise in:

Molecular Modeling:

- DFT Calculation, Bader Charge/Density of State Analysis, Thermal Correction, MKM, classical/ (QM/MM)/ab initio MD Simulation, TI/MTD Free Energy Calculation.

Programing:

- Python, Matlab, Fortran, Radial Distribution Function (RDF) Analysis, Machine Learning, NNPs.

Catalysis:

- Mechanistic Studies, Kinetic Modeling, Solvent Selection, Catalyst/Material Stability, Confinement and Entropy Quantification, Machine Learning, Neural Network Force Fields Development.

Software:

- Gaussian, CP2K, Quantum Espresso, VASP, LAMMPS, Amber, COMSOL, ASPEN, Solidwork, Packmol, VMD, MS Excel, MS Power Point, MS Word.

Experience in:

Experimental Technique:

- Scanning Electron Microscopy, Zetasizer, LUMiSizer, FTIR, X-ray Photoelectron Spectroscopy.

AWARDS AND HONORS

Presidential Award – NTU, Department of Chemical Engineering **2017**

- An award bestowed to the top 5% students in academic records.

Cathay Life Insurance Fellowship - **2016**

- Offered to students with an average score of A in academic record.

Taiwan Business Bank Fellowship - **2014**

- Offered to students with an average score of A in academic record.

PEER-REVIEWED PUBLICATIONS

- **Chen, T. H.**, Vlachos, D. G., & Caratzoulas, S. (2022) Computational Investigation of Pt Nucleation over γ-Al_2O_3 Surfaces and the Role of Hydroxylation and Sn. (In preparation)
- **Chen, T. H.**, Vlachos, D. G., & Caratzoulas, S. (2022) Ab initio Enhanced Sampling Study on Pd Nucleation over γ-Al_2O_3 Surfaces. (In preparation)
- Quiroz, N. R., **Chen, T. H.**, Chen, T. Y., Caratzoulas, S., & Vlachos, D. G. (2022) Unexpected Kinetic Solvent Effects Enhance Activity and Selectivity in Biphasic Systems. (Submitted)
- Luo, T. Y., Park, S., **Chen, T. H.**, Prerna, P., Patel, R., Siepmann, J. I., Caratzoulas, S., Xia, Z., & Tsapatsis, M. (2022). Simultaneously Enhanced Hydrophilicity and Stability of a Metal-Organic Framework via Post-Synthetic Modification for Water Vapor Sorption/Desorption. (Revised)
- **Chen, T. H.**, Vlachos, D. G., & Caratzoulas, S. (2021). Brønsted Acid Catalysis of the Direct Acylation of 2-Methylfuran by Acetic Acid. Theoretical Insights into the Role of Brønsted Acidity and Confinement. *ACS Catalysis*, 11(15), 9916-9925.
- Dorneles de Mello, M., Kumar, G., Tabassum, T., Jain, S. K., **Chen, T. H.**, Caratzoulas, S., ... & Tsapatsis, M. (2020). Phosphonate-Modified UiO-66 Brønsted Acid Catalyst and Its Use in Dehydra-Decyclization of 2-Methyltetrahydrofuran to Pentadienes. *Angewandte Chemie*, 132(32), 13362-13368.
- **Chen, T. H.,** Yeh, Y. C., & Liao, Y. C. (2018). Healable and foldable carbon nanotube/wax conductive composite. *ACS applied materials & interfaces*, 10(28), 24217-24223.

SELECTED CONFERENCE PRESENTATIONS

- **Chen, T. H.**, Vlachos, D. G., & Caratzoulas, S. (2022). Computational Insights into Pd Nucleation on γ-Al_2O_3 Surface. *27th North America Catalysis Society Meeting*. Poster
- **Chen, T. H.**, Vlachos, D. G., & Caratzoulas, S. (2020). Computational Insights into the Direct Acylation of 2-Methylfuran with Acetic Acid over Phosphotungstic Acid and H-BEA Zeolite. *AICHE Annual Meeting*. Presentation
- **Chen, T. H.**, Vlachos, D. G., & Caratzoulas, S. (2020). Acylation of 2-Methylfuran with Acetic Acid over HPW and H-BEA Catalyst. *CCEI Spring Symposium*. Presentation
- **Chen, T. H.**, & Liao, Y. C. (2017). Graphene-modified Sponges for The Oil Mist Removal. *Korea / Japan / Taiwan Chemical Engineering Conference*. Poster, First-Place Award
- **Chen, T. H.**, & Liao, Y. C. (2017). Fabrication of Healable Conductive Tracks on Foldable Substrates and Extremely Rough Surface with MWCNT-Based Composite. *Annual Meeting of Taiwanese Interface Society*. Poster, Third-Place Award

Yingjie Chen

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EDUCATION

University of Delaware Newark, DE
Ph.D. Candidate in Chemical and Biomolecular Engineering, GPA 3.66/4.00 08/2019 — 05/2023

Rutgers, The State University of New Jersey Piscataway, NJ
Ph.D. Student in Chemical and Biochemical Engineering, GPA 4.00/4.00 08/2018 — 08/2019

Rose-Hulman Institute of Technology Terre Haute, IN
B.S. in Chemical Engineering, magna cum laude, GPA 3.89/4.00 09/2014 — 05/2017

Nanyang Technological University Singapore
Chemical and Biomolecular Engineering, Global Exchange Program 01/2016 — 05/2016

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant 08/2018 — Present

Thesis Project: Modeling, Analysis, and Optimization of Continuous Pharmaceutical Manufacturing (CPM) Process under Industry 4.0 / Digital Twin Framework

Advisor: Prof. Marianthi Ierapetritou

- Participate in FDA-funded projects to realize digital twin framework for CPM processes under QbD initiative
- Establish mechanistic, data-driven multivariate, and hybrid models for unit operations to ensure predictability
- Develop physics-constrained neural network to integrate DEM with machine learning (ML/AI) framework
- Utilize data to conduct systems-based analyses in MATLAB/gPROMS to design control strategy
- Implement PAT chemometric models in Python for process monitoring and deploy them on cloud
- Collaborate with experimentalists to perform process optimization, reducing energy consumption by 80%
- Assess process environmental impacts with life cycle analysis to strive for process sustainability
- Extend feasibility-driven optimization with Gaussian Processes to multi-objective space for decision-making

ORISE Fellow 05/2022 — 08/2022

U.S. Food and Drug Administration (FDA), Center for Drug Evaluation and Research; ORAU/ORISE

- Performed data analytics research for process-induced API crystallinity/polymorphic change in manufacturing
- Surveyed over 4000 ANDAs/NDAs to identify industry CMC practices for polymorphic change
- Developed in-house statistical and population balance models (PBM) in Python to capture process CQAs

Operations Intern / Process Team Core Member 07/2017 — 08/2018

Eli Lilly and Company, Lilly Suzhou

- Coordinated cGMP process operations and cooperated with international sites to benchmark operation designs
- Integrated a data analysis platform with TrakSys using Python and VB to visualize process operations
- Acted as a core member in a Black Belt Six Sigma project to reduce batch changeover time from 4 to 2 hrs
- Implemented optimization measures (SOP, process, RCA, and HR) to improve shift effectiveness by 25%
- Contributed to change (MOC) and qualification (PQ) of speed-up projects to increase line capability by 50%
- Applied MES data to visually manage the shop floor, ensuring 100% on-time completion of plans

SKILLS

Software/Programming	Python, gPROMS, MATLAB, Aspen+, OSI PI, Rockwell PMX, TIBCO
Laboratory/Plant	Direct compaction, Wet granulation, Chromatography, Sterile filling, Packaging

PUBLICATIONS

1. **Chen, Y.,** Ding, C., Ierapetritou, M. (2022). "Surrogate-based multi-objective optimization with feasibility driven constraints for continuous pharmaceutical and biopharmaceutical manufacturing." [In Preparation].
2. **Chen, Y.**, Kotamarthy, L., Sampat, C., Dan, A., Bhalode, P., Singh, R., Glasser, B., Ierapetritou, M., Ramachandran, R. (2022). "Systems-based sensitivity analysis and optimization of key energy and performance metrics for pharmaceutical drug product manufacturing." Intl J. Pharmaceutics [Accepted].
3. **Chen, Y.,** Sampat, C., Huang, Y., Singh, R., Ramachandran, R., Reklaitis, G., Ierapetritou, M. (2022). "Implementation of data infrastructure for continuous pharmaceutical manufacturing." [In Preparation].
4. **Chen, Y.,** Gupta, S., Sampat, C., Ramachandran, R., Muzzio, F., Ierapetritou, M. (2022). "Adaptive NIRS model on an analytics platform for monitoring low dose blend uniformity in a feed frame." [In Preparation].
5. Sampat, C., Kotamarthy, L., Bhalode, P., **Chen, Y.**, Dan, A., Parvani, S., Dholakia, Z., Singh, R., Glasser, B., Ierapetritou, M., Ramachandran, R. (2022). "Enabling Energy-Efficient Manufacturing of Pharmaceutical Solid Oral Dosages via TEA and Process Modeling." J. Adv. Manuf. Process. e10136:1-20.
6. Bhalode, P., **Chen, Y.**, Ierapetritou, M. (2021). "Hybrid Modelling Strategies for Continuous Pharmaceutical Manufacturing within Digital Twin Framework." Comput. Aided Chem. Eng. 49:2125-2130.
7. **Chen, Y.**, Yang, O., Sampat, C., Bhalode, P., Ramachandran, R., Ierapetritou, M. (2020). "Digital Twins in Pharmaceutical and Biopharmaceutical Manufacturing: A Literature Review." Processes 8(9):1088.
8. **Chen, Y.**, Ierapetritou, M. (2020). "A framework of hybrid model development with identification of plant-model mismatch." AIChE Journal 66(10): e16996:1-16.

PRESENTATIONS

1. **Chen, Y.**, Bhalode, P., Ierapetritou, M. "Integration of High-Fidelity Simulation and Surrogate Modeling for Reduced Model Development in Continuous Pharmaceutical Unit Operations", AIChE, November 2022.
2. **Chen, Y.**, Gupta, S., Román-Ospino, A., Muzzio, F., Ierapetritou, M. "Adaptive Strategies for Updating Unit Operation Models and In-Line Monitoring of Blend Uniformity in CPM Process", AIChE, November 2021.
3. **Chen, Y.**, Ierapetritou, M. "Implementation of Hybrid Models to Perform System Analyses with Model Maintenance in Continuous Pharmaceutical Manufacturing", AIChE, November 2020.
4. **Chen, Y.**, Dias, L., Metta, N., Ierapetritou, M. "Data-driven Modeling of Unit Operations in Continuous Pharmaceutical Manufacturing Line under the Industry 4.0 Framework", ML in Science and Engr., June 2019.

TEACHING EXPERIENCE

Teaching Assistant, Dept. of Chemical and Biochemical Engineering, Rutgers 08/2018 — 08/2019

Courses: 155:415/416 Process Engineering Lab I/II (82 enrollment, with Prof. Alex Bertuccio)

· Coordinated the senior unit operations lab series and supervised all 13 laboratory experiments

ACTIVITIES

Vice President, Chemical and Biochemical Graduate Student Organization, Rutgers 09/2018 — 08/2019

Executive Member, Employee Wellbeing Team, Lilly 09/2017 — 07/2018

HONORS AND AWARDS

Nominated for the ORISE Future Science Award by FDA OPQ 2022

Travel Grant Award, 2019 Machine Learning in Science and Engineering Conference 2019

Best Operations Team Award; Best Team Award for Employee Wellbeing, Lilly 2018

Dean's List; Heminway Bronze Medal of Academic Superiority, Rose-Hulman 2014 — 2017

CHAOYING DING

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244 McFarland Dr
Newark, DE 19702

EDUCATION

University of Delaware — Newark, DE
Ph.D. Candidate in Chemical and Biomolecular Engineering, GPA 3.77/4.00 — 08/2019 — present

Tianjin University (Top 1 in Chemical Engineering in China) — Tianjin, China
M.S. in Chemical Engineering, GPA 3.6/4.0 — 09/2016 — 06/2019

Changzhou University — Jiangsu, China
B.S. in Chemical Engineering and Technology, GPA 4.4/5.0 — 09/2012 — 07/2016

Relevant courses: Convex optimization, Math modeling optimization, Separation technology, Biochemistry

RESEARCH EXPERIENCE

Graduate Research Assistant (For Ph.D. study) — 08/2019 — Present

Thesis Project: Modeling and optimization for advanced biopharmaceutical manufacturing

Advisor: Prof. Marianthi Ierapetritou

- Participate in FDA, NIIMBL, and industry funded projects in modeling, analysis, and optimization of batch and continuous biopharmaceutical manufacturing processes
- Develop mechanistic and hybrid models to simulate chromatographic elution behaviors in MATLAB / Python
- Calibrate and validate the developed chromatography models with process data from industry
- Utilize constrained sensitivity analysis to find the critical process parameters of chromatography
- Identify the design space of primary capture chromatography with a 36x reduction in computational time with the assist of machine learning (ML) techniques
- Conduct robustness analysis of the models and optimize chromatography performance under quality constraints
- Establish *in silico* batch and continuous platforms for the mAb production and plasma separation
- Perform scheduling analysis with the incorporation of the work shift and labor constraints to facilitate process debottlenecking and to accomplish continuous operations
- Employ techno-economic and environmental analysis to examine viability and cost-effectiveness of processes
- Evaluate the impacts of design variables by scenario analysis to reveal the flexibility of the developed platform

Graduate Research Assistant (For M.S. study) — 09/2016 — 06/2019

Lab of Advanced Nano-structures & Transfer Processes, Tianjin University

Advisor: Prof. Xiaobin Fan

- Developed novel hybrid nanomaterials/nanosheets by integrating transition metal oxides/sulfides and 2D materials with solvothermal, ball-milling, annealing, and salt molten method to facilitate charge delivery
- Investigated Li-ion battery storage mechanism and the enzymatic activity of immobilized lipase
- Characterized sample composition, structure, and bonding by Raman, XRD, XPS, SEM and TEM

SKILLS

Software/Programming Python, MATLAB / SIMULINK, SuperPro Designer, SchedulePro, gPROMS

Laboratory/Experiment XRD, TEM, SEM, Raman, UV-vis, FTIR, XPS, TGA, AFM, BET

PUBLICATIONS

1. **Ding, C.**, Chen, Y., Ierapetritou, M. (2022). "Constrained sensitivity analysis for the pharmaceutical and biopharmaceutical manufacturing." [In preparation]
2. **Ding, C.**, Ardeshna, H., Gillespie, C., Ierapetritou, M. (2022). "Process design of a fully integrated continuous biopharmaceutical process using economic and ecological impact assessment." Biotechnology and Bioengineering 119(12), 3567-3583.
3. **Ding, C.**, Ierapetritou, M. (2021). "A novel framework of surrogate-based feasibility analysis for establishing design space of twin-column continuous chromatography." International Journal of Pharmaceutics 609, 121161.
4. **Ding, C.**, Liang, J., Zhou, Z., Li, Y., Peng, W., Zhang, G., Zhang, F., Fan, X. (2019). "Photothermal enhanced enzymatic activity of lipase covalently immobilized on functionalized $Ti_3C_2T_X$ nanosheets." Chemical Engineering Journal 378, 122205.
5. Liang, J., **Ding, C.**, Liu, J. Chen, T., Peng, W., Li, Y., Zhang, F., Fan, X. (2019). " Heterostructure engineering of Co-doped MoS_2 coupled with Mo_2CT_X MXene for enhanced hydrogen evolution in alkaline media." Nanoscale 11 (22), 10992-11000.
6. **Ding, C.**, Qian, J., Li, Z., Li, Li, Y., Peng, W., Zhang, G., Zhang, F., Fan, X. (2018). "Cobalt phosphide nanoparticles anchored on molybdenum selenide nanosheets as high-performance electrocatalysts for water reduction." International Journal of Hydrogen Energy, 43(45), 20346-20353.
7. Jin, J., Liang, Q., **Ding, C.**, Li, Z., Xu, S. (2017) " Simultaneous synthesis-immobilization of Ag nanoparticles functionalized 2D g-C_3N_4 nanosheets with improved photocatalytic activity". Journal of Alloys and Compounds, 691, 763-771.
8. **Ding, C.**, Tian, L., Liu, B., Liang, Q., Li, Z., Xu, S., Liu, Q., Lu, D. (2015) "Facile in situ solvothermal method to synthesize MWCNT/$SnIn_4S_8$ composites with enhanced visible light photocatalytic activity". Journal of Alloys and Compounds, 633, 300-305.

PRESENTATIONS

1. **Ding, C.**, Ardeshna, H., Gillespie, C., Ierapetritou, M. "Process Design of a Fully Integrated Continuous Biopharmaceutical Process using Economic and Environmental Impact Assessment" (July 2022), NIIMBL Annual Meeting, Washington D.C.
2. **Ding, C.**, Ierapetritou, M. " Surrogate-Based Feasibility Analysis for the Identification of Design Space of Multicolumn Counter-Current Continuous Protein a Chromatography " (November 2021), AIChE Annual Meeting, Boston.

TEACHING EXPERIENCE

Teaching Assistant 09/2021 — 05/2022

CHEG 401 Chemcal Process Dynamics and Control (Prof. Ierapetritou and Prof. Ogunnaike, Enrollment: 91)

CHEG 112 Introduction to Chemical Engineering (Prof. Enszer and Prof. Blenner, Enrollment: 94)

· Responsible for recitations, office hours, laboratory instruction (via Simulink), and grading

HONORS AND AWARDS

First Prize of Undergraduate Excellent Thesis (Provincial-level, Top 10%, 05/2017)

First Prize of Higher Mathematics Competition in Jiangsu Province (Provincial-level, 06/2014)

National Scholarship (National-level, Top 1%, 11/2013)

Yagya Gupta

Email: yagya@udel.edu
Mobile: 302-898-8930

EDUCATION

University of Delaware (UD) — Delaware, U.S.A.
Ph.D. in Chemical Engineering — *Aug' 19 - present*

Guru Gobind Singh Indraprastha University (GGSIPU) — Delhi, India
Bachelor of Technology – Chemical Engineering — *Aug'15 – Jun'19*

PUBLICATIONS AND PATENTS

- Gupta, Y., Beckett, L. E., Sadula, S., Vlachos, D. G., Korley, L. T., *Bio-Based Polymers for the Purification of High Commercial Value Chemicals from Plants, Food Waste and Non-Food Biomass.* U. S. Patent 63/417,369 filed October 19, 2022. Provisional patent.
- Luo, Y., O'Dea, R.M., Gupta, Y., Chang, J., Sadula, S., Soh, L.P., Robbins, A.M., Levia, D.F., Vlachos, D.G., Epps III, T.H. and Ierapetritou, M., A Life Cycle Greenhouse Gas Model of a Yellow Poplar Forest Residue Reductive Catalytic Fractionation Biorefinery. Environmental Engineering Science, 2022
- Ebikade, E.O., Sadula, S., Gupta, Y., and Vlachos, D.G. A Review of Thermal and Thermocatalytic Valorization of Food Waste. Green Chemistry, 2021
- Gupta, Y., Bhattacharyya, S., and Vlachos, D.G. Extraction of Valuable Chemicals from Food Waste via Computational Screening and Experiments. (Submitted)
- Gupta, Y., Beckett, L. E., Sadula, S., Vargheese, V., Korley, L. T., Vlachos, D.G., Development and Application of Bio-based Polymers for the Selective Separation and Purification of High Commercial Value Chemicals Extracted from Food Waste, Plants and Non-Food Biomass. (Under Preparation)

RESEARCH EXPERIENCE

Valorization of Food Waste to Produce High Commercial Value Chemicals

Jan'20 - present

- Optimized the selective extraction of phenolics from different food waste feedstocks using thermodynamic models (COSMO-RS and HSPiP) to guide the experimental design
- Developed and optimized microwave-assisted extraction of key phenolics from mixed food waste
- Developed a new separation methodology using biobased polymers for purification of the target phenolics after extraction, up to 8 times more economical than the current industrial method

Production of Dimethyl Terephthalate from Biomass-Derived Platform Molecule

Sept'18 – May'19

- Optimized the retro-Diels alder (rDA) reaction to produce dimethyl terephthalate using Density Functional Theory (DFT)
- Experimentally investigated and optimized the production of dimethyl terephthalate from biomass-derived platform molecule

Synthesis of Carbon-Free Proton Exchange Membrane Fuel Cell Catalyst Supports

Jun' 18 – Aug'18

- Investigated the performance of four antimony-doped tin oxide supports treated with different amounts of carbon and silica
- Studied the support microstructure using transmission electrode microscopy (TEM), scanning electron microscopy (SEM), and Brunauer-Emmet-Teller (BET) analyzer for nitrogen gas sorption

- Studied the electrochemical properties of the synthesized supports using the rotating disk electrode (RDE) test

Development of an Alternate Biobased Route to Produce High Commercial Aromatic Compounds from 2-pyrone

Jan'18 to Mar'18

- Performed Density Functional Theory (DFT) simulations to optimize the retro-diels alder reaction of 2-pyrone obtained from the fermentation of biomass to commercially aromatic compounds
- Investigated the reaction mechanism and stability in four solvents

AWARDS AND HONORS

- Elected as the chair of Gordon Research Seminar on Chemical Separations, 2024 *2022*
- Travel Award, Gordon Research Conference on Chemical Separations *2022*
- Awarded 1st prize in the 7th Annual DENIN research poster competition, Delaware Environmental Institute (DEI) *2022*
- Awarded the gold medal for academic excellence, GGSIPU *2019*
- Received recognition for holding department rank 1 consistently for four years, GGSIPU *2019*
- Received Best Innovation Award in Chem-E-car competition, IIT-BHU *2017*

CONFERENCE PRESENTATIONS

- "Separation and Purification of High-Value Chemicals Extracted from Food Waste," American Institute of Chemical Engineers (AIChE) Annual Meeting, Phoenix, U.S.A. *Nov'22*
- "Separation and Purification of High-Value Chemicals Extracted from Food Waste," *poster presentation*, Gordon Research Conference/ Seminar on Chemical Separations, Ventura, U.S.A. *Oct'22*
- "Solvent Optimization for Extraction of High Commercial Value Chemicals from Food Waste," *poster presentation*, 27th North American Catalysis Society Meeting, New York City, USA *May'22*
- "Solvent Optimization for Extraction of High Commercial Value Chemicals from Food Waste," American Institute of Chemical Engineers (AIChE) Annual Meeting, Boston, USA *Nov'21*
- "Solvent Optimization for Extraction of High Commercial Value Chemicals from Food Waste," 25th Annual Green Chemistry and Engineering Conference *Jun'21*
- "Synthesis of Carbon Free Fuel Cell Catalyst Supports," *poster presentation*, American Institute of Chemical Engineers (AIChE) Annual Meeting, Pittsburgh, U.S.A. *Oct'18*
- "E-Waste to Z-waste," *poster presentation*, American Institute of Chemical Engineers (AIChE) Annual Meeting, Minneapolis, U.S.A. *Oct'17*

MENTORSHIP AND LEADERSHIP EXPERIENCE

- President, Indian Graduate Student Association at UD *May'22 – Apr'23*
- Lead Mentor, EmPOWER mental health and peer-support Group at UD *Oct'22 – Sept'23*
- Mentored 1 undergraduate researcher at UD: Brian Barrett *Nov'21 – present*
- Student Mentor, EmPOWER mental health and peer-support Group at UD *Oct'21 – Sept'22*
- Department representative, Women in Engineering group at UD *May'20 – present*
- Academic School Representative of my department at GGSIPU *Aug'18 – May'19*
- Vice President of the Publication Club at GGSIPU *Aug'18 – May'19*
- Editor-in-chief of the Publication Club at GGSIPU *Aug'17 – May'18*

Kentaro Hansen

PhD Candidate, Graduate Research Assistant
University of Delaware, Department of Chemical & Biomolecular Engineering.
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https://orcid.org/0000-0001-7519-1655
https://www.linkedin.com/in/kentaro-hansen-30b232191/

Research Statement

PhD. Candidate in Chemical Engineering with a focus on the engineering of electrochemical devices. My work has focused on developing a diagnostic technique to deconvolute individual electrode and membrane contributions to cell overpotential and internal resistance as well as advanced electrochemical cell designs for anion-exchange and bipolar/double membrane-based devices. I have worked on a U.S. Department of Energy grant focused on developing and scaling a double-membrane electrochemical cell to produce formic acid from CO_2 and have worked on topics including quasi-reference electrodes, electrochemical impedance spectroscopy, techno-economic analysis, and life cycle inventory assessments.

Education

2019-present	**PhD. in Chemical & Biomolecular Engineering**, University of Delaware, Newark, DE. Thesis: Deconvolution of Energetic Losses in scalable membrane-based electrochemical devices Thesis Advisor: Prof. Feng Jiao GPA: 3.76
2015-2018	**B.S. in Chemical Engineering**, Rensselaer Polytechnic Institute, Troy, NY. GPA: 3.85

Research Experience

2019-present	**Graduate Research Assistant**, University of Delaware, Department of Chemical & Biomolecular Engineering Research focus: Deconvolution of Energetic Losses in a CO_2 Electrolyzer Advisor: Prof. Feng Jiao -Designed and completed experiments related to hot-pressing techniques for catalyst coating anion-exchange membranes -Mentored and trained junior students, including undergraduate and graduate students -Completed technoeconomic and life cycle inventory assessments of electrochemical CO_2 utilization technologies -Designed and assembled auxiliary equipment including temperature control units, humidifiers, Potentiostat multiplexers, and serial port communication interfacing with Arduino IDE, Matlab, and potentiostat software.
2019 Summer	**Research Intern**, Massachusetts Inst. Of Technology Lincoln Lab, Group 47 Research focus: Detection and attribution of post blast explosive debris Advisor: Dr. Joshua Dettman

-Methodology development for extraction and quantitation of trace explosive compounds from sediment (clay, silt, sand)

2019 Spring **DOE SULI Research Intern**, Lawrence Berkeley National Lab, Energy Conversion Group
Research focus: Water uptake properties of partially-exchanged Ce^{3+} doped Nafion thin films (20-200 nm)
Advisor: Dr. Ahmet Kusoglu
-Methodology development for partial doping of ionomer thin films and quantitation via 2D-XRF.

2018 Summer **Research Intern**, WL. Gore & Associates, Fuel Cell Technologies
Research focus: Measurement of proton exchange membrane (PEM) transport properties and statistical validation
Advisor: Dr. Erin Setzler
- Conducted a design of experiment and then statistically validated a test method for measuring water diffusion through PEMs.
-Measured metal ion loading in various thickness PEMs to quantitate in-plane cation doping variability.

Publications

First Author Publications

1. **Hansen, K. U.**, Cherniack L.H., and Jiao, F. "Voltage loss diagnosis in CO_2 electrolyzers using five-electrode technique." *ACS Energy Letters* 7 (2022): 4504-4511.
2. Haeun, S.*, **Hansen, K. U.***, and Jiao, F. "Techno-economic assessment of low-temperature carbon dioxide electrolysis." *Nature Sustainability* 4.10 (2021): 911-919. **(co-first author)**

Co-author Publications

3. Stephens, I. E., **et al.** "2022 roadmap on low temperature electrochemical CO_2 reduction." *Journal of Physics: Energy* 4.4 (2022): 042003.
4. Redmond, E. L., **Hansen, K. U.**, and Berg, D. W. "Development of Water Vapor Transport Resistance Protocol and Analysis." *ECS Transactions* 92.8 (2019): 445.

Non peer-reviewed Publications and Reports

5. **Hansen, K. U.**, and Jiao, F. "Creating the right environment." *Nature Energy* 6.11 (2021): 1005-1006.
6. **Hansen, K. U.**, and Jiao, F. "Hydrophobicity of CO2 gas diffusion electrodes." *Joule* 5.4 (2021): 754-757.
7. **Hansen K. U**., and Jiao, F. "Electrochemical Conversion of Carbon dioxide to Alcohols LCA Report." *U.S. DOE,* NETL. (2020). (Commissioned for U.S. Department of Energy, National Energy Technology Laboratory to satisfy award requirements for Award No. DE-FEE0029868.)

Presentations

2022 241st ECS Meeting, Vancouver, BC, Canada
Deconvoluting CO_2 Electroreduction Membrane-Electrode-Assembly Performance Via Five-Electrode Setup.

Academic Work Experience

Spring 2021 **Graduate Teaching Assistant**, University of Delaware, Department of Chemical & Biomolecular Engineering
Responsibilities: Assigning and grading interim assessments, holding office hours, and formulating grading rubrics for the interim and final assessment.
Supervisors: Prof. Feng Jiao, Prof. Yushan Yan

Honors and Awards

2018 **Coonley Prize** Rensselaer Polytechnic Institute, Howard P. Isermann Department of Chemical and Biological Engineering
Awarded for best senior design project

2017 **AIChE ChemE Car Northeast Competition 2nd place**
Acted as team engineering lead, enabling team to compete at national level, first time in nine years for undergraduate team.

2015 **Rensselaer Leadership Award**
Academic scholarship awarded for duration of undergraduate studies awarded prior to matriculation

Skills

Programming skills (Matlab): serialport communication, GUI development, fitting and statistical analysis, technoeconomic modeling, image processing (e.g., pressure paper mapping)

Computational programs: ASPEN Modeling, Minitab, JMP, OriginLab, Arduino IDE, vector graphics design software (Affinity Designer)

Laboratory techniques: membrane electrode assembly preparation, electrochemical experiments, electrochemical impedance spectroscopy, equipment construction and maintenance, potentiostat multiplexing, reactor design and manufacturing, laser cutting, material characterization (HPLC, XRF, SEM EDX, GC-MS, ICPMS)

Mi Jen Kuo

mjkuo@udel.edu, +1(626) 371-6107

Education

University of Delaware, Newark, DE
- Ph.D. Candidate in Chemical and Biomolecular Engineering 2019 - Present

National Tsing Hua University, Hsinchu, Taiwan
- B.S. in Chemical Engineering 2015 - 2019

Experience

Graduate Research Assistant, University of Delaware 2019 - Present

Advisor: Dr. Raul F. Lobo. Selected research projects:
- Green Synthesis of 4,4'-dimethylbiphenyl (DMBP) from Biomass
  - Developed a green synthesis route for DMBP as a platform chemical for polymers
  - Optimized the yield of DMBP using design of experiments methodology
- Two-step Synthesis of a Bisphenol-A Substitute from Biomass
  - Synthesized a diol molecule through oxidative coupling and hydrogenation from biomass-derived furfuryl acetate
  - Designed an effective separation process to obtain the diol molecule with high purity
- Oxidative Dehydrogenation of Ethane using Zeolite-Supported Catalysts
  - Synthesized and characterized molecular sieve catalysts
  - Achieved excellent ethane conversion and ethylene selectivity

Leadership

Chemical Engineering Student Chapter President, **National Tsing Hua University** 2017 - 2018
- Lead the student chapter and represented the undergraduate student population
- Organized social, educational, and career events for the students

Skills

- **Lab:** XRD, SEM/EDS, TGA, XRF, UV-Vis Spectroscopy, Physisorption/ Chemisorption Analyzer, Liquid and Solid-state NMR, GC, HPLC, LC-MS
- **Software:** Microsoft Office, Minitab, MATLAB, Aspen, Origin

Publications and Presentations

Journal Articles
- Cho, H. J.; **Kuo, M. J.** (co-first author); Ye, M.; Kurz, Y.; Yuan, Y.; Lobo, R. F. Selective Synthesis of 4,4'-Dimethylbiphenyl from 2-Methylfuran. *ACS Sustain. Chem. Eng.* **2021**, *9* (8), 3316–3323.
- Luo, Y.; **Kuo, M. J.** (co-first author); Ye, M.; Lobo, R.; Ierapetritou, M. Comparison of 4,4'-Dimethylbiphenyl from Biomass-Derived Furfural and Oil-Based Resource: Technoeconomic Analysis and Life-Cycle Assessment. *Ind. Eng. Chem. Res.* **2022**, *61* (25), 8963–8972.
- Ye, M.; **Kuo, M. J**.; Lobo, R. F. Oxidative Coupling of 2-Methyl Furoate: A Scalable Synthesis of Dimethyl 2,2'-Bifuran-5,5'-Dicarboxylate. *Appl. Catal. A Gen.* **2021**, *619* (March), 118138.

Conference Presentations
- **Kuo, M. J**.; Cho, H.J.; Lobo, R. F. Synthesis of Bio-Sourced 4,4'-Dimethylbiphenyl. 2021 AIChE Annual Meeting.

Shizhao Lu

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EDUCATION

University of Delaware, Newark, DE — Sept. 2019 - May 2024 (Anticipated)
Ph.D. Chemical & Biomolecular Engineering

University of Pennsylvania, Philadelphia, PA — Sept. 2017 - June. 2019
M.S.E. Chemical & Biomolecular Engineering

Nanjing Tech University, Nanjing, China — Sept. 2013 - June. 2017
B.S. Chemical Engineering

RESEARCH EXPERIENCE

Ph.D. Researcher — Sept. 2019-Present

University of Delaware, Newark, DE
Thesis Advisor: Prof. Arthi Jayaraman

Thesis Title: Molecular modeling, simulation and machine learning of polymer nanocomposites containing nanorod fillers

- Developed coarse-grained molecular models to capture the effect of chemical and physical heterogeneity of nanorods on nanorod morphology in polymer nanocomposites
- Developed a semi-supervised machine learning workflow for label-efficient, automatic classification and segmentation of protein nanowire morphologies from transmission electron microscopy (TEM) images and demonstrated the transferability of the workflow on other TEM image datasets for morphology classification
- Developing variational autoencoders to generate nanowire morphology images with specified nanowire pixel fraction and fractal dimension
- Collaborated in multi-functional project for design and synthesis of next generation bio-material protein / peptide nanowires for renewable soft electronics

Interdisciplinary Machine Learning Hackathon Project — Feb. 2022-May. 2022

University of Delaware, Newark, DE
Course Advisor: Prof. Arthi Jayaraman and Prof. Sunita Chandrasekaran
Industry Mentor: Dr. Houk Jang from NIST

- Developed machine learning models to determine the degree of blurriness of optical microscopy images containing metal flakes with convolutional neural networks (CNNs)
- Communicated bi-weekly to an industrial mentor in an interdisciplinary team consisting of students from chemical engineering, material science, chemistry, computer science and data science

Graduate Researcher — Nov. 2017-Feb. 2019

University of Pennsylvania, Philadelphia, PA
Research Advisor: Prof. Daeyeon Lee

Photochemical stability of Poly(methyl methacrylate) (PMMA) confined in nanocomposite

- Assembled polymer nanocomposite film by Capillary Rise Infiltration (CaRI) technique
- Utilized spectroscopic ellipsometry and UV-Vis spectroscopy to study the photochemical stability of PMMA in composite film

Polymer adsorption on stainless steel coating

- Conducted *in-situ* measurement of polymer adsorption in a liquid cell using Quartz Crystal Microbalance with Dissipation (QCM-D)
- Estimated the volume fraction of polymer in the adsorbed polymer layer

LEADERSHIP EXPERIENCE

Teaching Assistant — Aug. 2020-May. 2021

University of Delaware, Newark, DE

- Assisted professors in teaching graduate level statistics and design of experiment
- Managed 8 groups of 4-5 senior undergraduate students in a distillation lab course on ASPEN and DCS virtual lab simulations

SKILLS

- Professional skills: Microsoft Word, Excel, Powerpoint, Endnote
- Modeling and simulation skills: Coarse-grained modeling, molecular dynamics simulations
- Software: Python, Tensorflow, LAMMPS, VMD, MATLAB, ASPEN, bash scripting, high-performance-computing on supercomputer clusters
- Machine learning skills: computer vision, image-based deep learning, semi-supervised learning, self-supervised learning, variational autoencoders
- Experimental techniques: HPLC, QCM-D, spectroscopic ellipsometry, UV-Vis
- Languages: English (Fluent), Mandarin (Native)

PUBLICATIONS

- **Lu, S.**, Jayaraman, A. Application of Variational Autoencoders for Generation of Nanowire Morphology Images. *(In preparation)*
- **Lu, S.**, Montz, B., Emrick, T. and Jayaraman, A. Semi-supervised Machine Learning Workflow for Analysis of Nanowire Morphologies from Transmission Electron Microscopy Images. *Digital Discovery* **2022** DOI: 10.1039/D2DD00066K
- **Lu, S.**, Jayaraman, A. Effect of Nanorod Physical Roughness on the Aggregation and Percolation of Nanorods in Polymer Nanocomposites. *ACS Macro Lett* **2021**, 10 (11), 1416-1422. DOI: 10.1021/acsmacrolett.1c00503.
- **Lu, S.#**, Wu, Z.#, Jayaraman, A. Molecular Modeling and Simulation of Polymer Nanocomposites with Nanorod Fillers. *The Journal of Physical Chemistry B* **2021**, *125* (9), 2435-2449. DOI: 10.1021/acs.jpcb.1c00097
- Xue, F., Xu, Y., **Lu, S.**, Ju, S. and Xing, W. Adsorption of Cefocelis Hydrochloride on Macroporous Resin: Kinetics, Equilibrium, and Thermodynamic Studies. *Journal of Chemical & Engineering Data*, **2016**. *61*(6), pp.2179-2185.

CONFERENCE PRESENTATIONS

- **Lu, S.**, Jayaraman, A. Semi-Supervised Machine Learning Workflow for Analysis of Nanostructured Morphologies from Transmission Electron Microscopy Images. (Talk) MRS Fall Meeting, Boston, MA, 2022
- **Lu, S.**, Molecular Modeling, Simulation, and Machine Learning of Polymer Nanocomposites Containing Nanowire and Nanorod Fillers. (Poster) Summer Research Review, Department of Chemical & Biomolecular Engineering, University of Delaware, Newark, DE, 2022
- **Lu, S.**, Jayaraman, A. Effect of Nanorod Physical Roughness on the Aggregation and Percolation of Nanorods in Polymer Nanocomposites. (Talk) APS March Meeting, Chicago, IL, 2022
- **Lu, S.**, Coarse-Grained Modeling and Simulation Studies of Polymer Nanocomposites Containing Nanorod Fillers. (Talk) Summer Research Review, Department of Chemical & Biomolecular Engineering, University of Delaware, Newark, DE, 2021
- **Lu, S.#**, Wu, Z.#, Jayaraman, A. Coarse-grained Models for Predicting the Morphology of Polymer Nanocomposites Containing Nanorod Fillers. (Talk) APS March Meeting (virtual) 2021
- **Lu, S.#**, Wu, Z.#, Jayaraman, A. Coarse-grained Models for Predicting the Morphology of Polymer Nanocomposites Containing Nanorod Fillers. (Talk) AIChE Annual Meeting (virtual) 2020

OPEN-ACCESS CODE & DATASET DEVELOPED

- Semi-Supervised Machine Learning Workflow for Analysis of Nanowire Morphologies from TEM Images https://github.com/arthijayaraman-lab/semi-supervised_learning_microscopy_images
- Transmission Electron Microscopy (TEM) Image Datasets of Peptide / Protein Nanowire Morphologies https://doi.org/10.5281/zenodo.7025602
- Autofocusing Optical Microscope using Artificial Neural Network for Large-Area, High-Magnification Scanning https://github.com/evanmacbride/microscope-autofocus

AWARDS & HONORS

- First Prize in the National Chemical Design Competition 2016
- Merit Student of Nanjing Tech University 2015
- Celanese Outstanding Engineer Scholarship 2014

Yuqing (Robert) Luo

Email: yqluo@udel.edu| Mobile: 302-250-0685| LinkedIn: www.linkedin.com/in/yqluo

EDUCATION

University of Delaware, Newark, DE 08/2019 – Present
Ph.D. Candidate in Chemical and Biomolecular Engineering, GPA 4.00/4.00

University of Pennsylvania, Philadelphia, PA 07/2018 – 12/2018
Visiting Research Student in Prof. Virgil Percec's group (*Living radical polymerization kinetics*)

Shanghai Jiao Tong University, Shanghai, China 09/2015 – 07/2019
Bachelor of Science in Macromolecule (Applied Chemistry), GPA 4.02/4.30

RESEARCH EXPERIENCE

Graduate Research Assistant 11/2019 – Present

Thesis Project: Techno-economic Analysis (TEA) and Life Cycle Assessment (LCA) of Chemical Production from Biomass Feedstocks

Advisor: Prof. Marianthi Ierapetritou

Participate in DOE's RAPID, NSF GCR, and NSF EPSCoR projects for sustainable biomass conversion process simulation, evaluation, and integrated biorefinery/supply chain design.

- Optimize technology and feedstock choices for biorefinery under price/demand/supply/yield uncertainty using superstructure-based stochastic programming.
- Build neural network surrogate models in Python for process flexibility, and embed surrogate flexibility requirement in GAMS model.
- Formulate a modular supply chain model for biomass conversion facilities in the Baltimore-Wilmington-Philadelphia region in consideration of supply and demand variability.
- Optimize facility locations, transportation, and inventory level over 12 months through rolling horizon planning (connecting MATLAB and GAMS).
- Compare the cost/emission of 4,4'-Dimethylbiphenyl (DMBP) production from toluene and from sustainable furfural through Aspen Plus flowsheet simulation.
- Illustrate 40% less CO_2 emission but 18% more production cost in furfural-based DMBP production and revealed its bottlenecks.
- Integrate process design, simulation, and Bayesian optimization to find optimal hydrodeoxygenation reaction conditions that reduce 25% of global warming potential (GWP) and production cost.
- Perform TEA on process-intensified lignin depolymerization based on Aspen Plus simulation, demonstrating a 4%-62% reduction in cost as compared to the conventional technology.
- Develop the PET waste glycolysis flowsheet that produces the intermediate (BHET) with an 85% reduction in GWP and a 14%-56% decrease in cost.
- Design the PP waste hydrogenolysis process to make lubricant at a comparable cost but with 67% lower GWP and 40% energy usage than the Group III lubricants.

TEACHING EXPERIENCE

- CHEG 431 Chemical Process Analysis (Fall 2021, with Prof. Yushan Yan): Product and process design
- CHEG 841 (Spring 2021, with Prof. Babatunde Ogunnaike): Probability and statistics for engineers

HONORS AND AWARDS

Foundations of Computer Aided Process Operations/Chemical Process Control Travel Award	2023
Collins Fellowship: Department of Chemical and Biomolecular Engineering, University of Delaware	2020
Shanghai Outstanding Graduate (Top 5%): Shanghai Education Commission	2019
National Scholarship (Top 1%): Ministry of Education, China	2016

SKILLS

Software/Programming: Python, MATLAB, ASPEN PLUS, GAMS, SimaPro, Minitab, TensorFlow, Scikit-learn, Mixed integer (non)linear programming, supply chain optimization, stochastic programming

Laboratory: (Stress-controlled & Strain-controlled) Rheometer, GPC, NMR, Living-radical polymerization

PUBLICATIONS

1. Wang, Z., **Luo, Y.,** Wang, Y., Athaley, A., Chen, T., Ierapetritou, M., Vlachos, D.G., Water Effect in the Hydrodeoxygenation of 5-Hydroxymethylfurfural: A Biorefinery Process Integration and Optimization Perspective, ***in preparation***.
2. **Luo, Y.,** Selvam, E., Vlachos, D.G., Ierapetritou, M., Economic and Environmental Benefits of Modular Microwave-assisted PET Depolymerization, ***in revision***.
3. **Luo, Y.**, Ierapetritou, M., Multi-feedstock and Multi-product Process Design using Neural Network Surrogate Flexibility Constraints. *Industrial & Engineering Chemistry Research,* ***in revision***.
4. **Luo, Y.,** O'Dea, R. M.; Gupta, Y; Chang, J.; Sadula, S.; Soh, L.; Robbins, A. M.; Levia, D. F.; Vlachos, D.G.; Epps, T. H., III; Ierapetritou, M., A Life Cycle Greenhouse Gas Model of a Yellow Poplar Forest Residue Reductive Catalytic Fractionation Biorefinery. *Environmental Engineering Science*, **2022**, *39*(10), 821-833.
5. **Luo, Y.**, Ierapetritou, M., Uncertainty Evaluation of Biorefinery Supply Chain's Economic and Environmental Performance Using Stochastic Programming. *Computer Aided Chemical Engineering,* **2022**, *49*, 481-486.
6. **Luo, Y.**[†], Kuo, M. J.[†], Ye, M., Lobo, R. and Ierapetritou, M., Comparison of 4,4'-Dimethylbiphenyl from Biomass-Derived Furfural and Oil-Based Resource: Technoeconomic Analysis and Life-Cycle Assessment. *Industrial & Engineering Chemistry Research*, **2022**, *61* (25), 8963–8972
7. O'Dea, R. M.[†], Pranda, P.[†], **Luo, Y.**[†], Amitrano, A., Ebikade, E., Gottlieb, E., Ajao, O., Benali, M., Vlachos, D., Ierapetritou, M., and Epps, T. H., III, Ambient-pressure Lignin Valorization to High-performance Polymers by Intensified Reductive Catalytic Deconstruction. *Science Advances,* **2022**, *8* (3), eabj7523.
8. **Luo, Y.,** O'Dea, R., Epps, T. H., III, Ierapetritou, M., Comparative Study of Different Hybrid Life Cycle Assessment Methodologies Applied to Biomass-based Chemical Production. *Computer Aided Chemical Engineering*, **2021**, *50*, 1683-1688
9. **Luo, Y.**, Ierapetritou, M., Comparison between Different Hybrid Life Cycle Assessment Methodologies: A Review and Case Study of Biomass-based *p*-Xylene Production. *Industrial & Engineering Chemistry Research*, **2020**, *59* (52), 22313–22329
10. Feng, X., Maurya, D., Bensabeh, N., Moreno, A., Oh, T., **Luo, Y.,** Lejnieks, J., Galia, M., Miura, Y., Monteiro, M., Lligadas, G., Percec, V., Replacing Cu(II)Br_2 with Me_6-TREN in Biphasic Cu(0)/TREN Catalyzed SET-LRP Reveals the Mixed-Ligand Effect. *Biomacromolecules*, **2019**, *21* (1), 250–261

CONFERENCE PRESENTATIONS

1. **Luo, Y.,** Ierapetritou, M., Surrogate-based Optimization of a Flexible Integrated Biorefinery. Foundations of Computer Aided Process Operations/Chemical Process Control (FOCAPO/CPC 2023), San Antonio, **2023**
2. Liu, Y., **Luo, Y.,** Anastasopoulou, A., Ierapetritou, M., Environmental and Economic Analysis of the Polyethylene Terephthalate Production from Biomass-based *p*-Xylene. (FOCAPO/CPC), San Antonio, **2023**
3. **Luo, Y.,** Selvam, E., Vlachos, D.G., Ierapetritou, M., Techno-Economic Analysis and Life Cycle Assessment of Modular Microwave-Assisted PET Depolymerization. AIChE Annual Meeting, Phoenix, **2022**
4. **Luo, Y.,** Ierapetritou, M., Multi-Objective Optimization of Flexible Integrated Biorefinery Design. AIChE Annual Meeting, Phoenix, **2022**
5. Selvam, E., **Luo, Y.**, Ierapetritou, M., Lobo, R.F., Vlachos, D.G., Microwave-assisted depolymerization of PET over heterogeneous ZnO Catalysts. 2nd International Conference on Unconventional Catalysis, Reactors & Applications (UCRA 2022), Warwick, UK **2022**
6. **Luo, Y.**, Ierapetritou, M., Integrated Biorefinery Design Under Multi-Scale Uncertainties. AIChE Annual Meeting, Boston, **2021**
7. **Luo, Y.**, O'Dea, R., Epps, T. H., III, Ierapetritou, M., Process design and techno-economic analysis of pressure-sensitive adhesive polymer production from lignin. 25th Annual Green Chemistry & Engineering Conference, **2021**

ACTIVITIES

Colburn Club At-Large representative: Department of Chemical and Biomolecular Engineering (UD) 2021
Coordinator of weekly biomass and waste plastic conversion meetings between experimental and modeling teams for the Rapid Advancement in Process Intensification Deployment (RAPID) group at UD 2021

Nicholas Joseph Oliveira

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Elkton, MD 21921

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www.linkedin.com/in/NJOliveira

Education

University of Delaware **August 2018-Present**
Ph.D. Chemical Engineering

University of Connecticut **August 2013-May 2018**
B.S. Honors Chemical Engineering
B.A. German Language

Experience

The Bingjun Xu and Yushan Yan Labs **January 2019-Present**

- Spectro-electrochemical techniques to study Hydrogen oxidation and CO reduction mechanisms
- Optimization of a state-of-the-art continuous electrochemical CO_2 removal device

UCONN Research Assistant: The Willis Lab **August 2015–May 2018**

- Developed models to simulate light waves in dielectric media for high efficiency lighting
- Designed a prototype spatial ALD device for electrochemical and solar devices

Fraunhofer Institute for Solar Energy Systems **March 2017-August 2017**

- Tested various materials to prevent Bipolar Plate corrosion in Fuel Cell Stacks
- Designed test apparatus to measure corrosion through electrochemical fundamentals

MSU Research Assistant (REU Student): **May 2015 – August 2015**

- Received National Science Foundation funding for computational and experimental research in grain growth and the mechanical properties of compacted powdered steel (FC-0205)

Teaching Experience

GAANN ITChE Teaching Fellow **January 2022 – December 2022**

- Mentoring on teaching techniques and opportunities teaching undergraduate classes

Thermodynamics I **Fall 2020**

- 4 hours of office hours/week lecturing and reviewing material from class

Process Control **Fall 2019**

- 2 hour office hours and developed process design labs using MATLAB Simulink

Junior Lab **Spring 2018**

- Undergraduate TA experience, redesigning hands-on reactor modeling labs

Peer-Reviewed Publications

1. Rebollar, L., Intikhab, S., **Oliveira, N. J.**, Yan, Y., Xu, B., McCrum, I. T., Snyder, J. D. & Tang, M. H. “Beyond adsorption” descriptors in hydrogen electrocatalysis. *ACS Catal.* **10**, 14747–14762 (2020).
2. Malkani, A. S., Li, J., **Oliveira, N. J.**, He, M., Chang, X., Xu, B. & Lu, Q. Understanding the electric and nonelectric field components of the cation effect on the electrochemical CO reduction reaction. *Sci. Adv.* **6**, (2020).
3. Yang, X., Nash, J., **Oliveira, N. J.**, Yan, Y. & Xu, B. Understanding the pH Dependence of Underpotential Deposited Hydrogen on Platinum. *Angew. Chemie - Int. Ed.* **58**, 17718–17723 (2019).
4. Chang, X., Vijay, S., Zhao, Y., **Oliveira, N.**, Chan, K., and Xu, B. Understanding the Complementarities of Surface-Enhanced Infrared and Raman Spectroscopies in CO

Nicholas Joseph Oliveira

101 Dennis Drive
Elkton, MD 21921

(860) 249-4303
Njo@udel.edu
www.linkedin.com/in/NJOliveira

Adsorption and Electrochemical Reduction. *Nature Communications* Accepted

Conference Presentations

1. **Nicholas J Oliveira**, Yushan Yan, Evidence for Caffeine's Positive Impact on HOR/HER Activity through Water Rearrangement As Opposed to Direct Influence on the Interfacial Electric Field 2022 *Meet. Abstr.* **L03-2157**
2. **Nicholas J Oliveira**, Bingjun Xu, and Yushan Yan, Evidence for the Lack of Caffeine Specific Adsorption and Its Impact on Water Structure to Increase HOR/HER Activity on Pt 2021 *Meet. Abstr.* **MA2021-02 1484**
2. **Nicholas J Oliveira**, Arnav Malkani, Bingjun Xu, and Yushan Yan, Understanding Electric and Non-Electric Field Effects on Electrochemical Double Layer Restructuring for the Model Platinum HOR 2020 *Meet. Abstr.* **MA2020-02 3161**

Awards

Robert L. Pigford Fellow **August 2018-July 2019**
Graduate school year 1 fellowship

GAANN ITChE Fellow **January 2022 – December 2022**
Graduate teaching fellowship

Organizations

The Electrochemical Society
Member

EmPOWER Mentor University of Delaware
Mentor promoting awareness of mental health issues in graduate school

Colburn Club University of Delaware
Professional organization for graduate chemical engineering students. Positions held: Outreach coordinator, vice president, and 4th year representative
Middle School Mathematics Tutor

Alexandra Oliveira

Elkton, MD 21921
(860) 990-3520 ● amolive@udel.edu ● www.linkedin.com/in/alexmoliveira

Education

University of Delaware, Newark, DE *Expected: May 2024*
- Ph.D. Candidate in Chemical Engineering

University of Connecticut, Storrs, CT *May 2019*
- B.S.E. in Chemical Engineering, Summa Cum Laude, Minor: English
- Cumulative GPA: 3.97/4.00, Honors Program, Nutmeg Scholar, Deans List (Fall Spring 2019)

Research Experience

Yan Lab at University of Delaware, Newark, DE *January 2020-Present*
Graduate Research Assistant, Lab Manager
- Optimized anion exchange membrane (AEM) electrolyzer performance and improved energy efficiency through design of porous electrodes and study of operational parameters
- Synthesized electrocatalysts through electroless and electrodeposition mechanisms and tested half-cell catalyst activity through electrochemical methods
- Mentored an undergraduate researcher in the experimental optimization of ionomer incorporation for high-performance electrolyzers
- Studied CO_2 contamination mechanisms, chloride contamination, and water transport in AEM electrolyzers through experiments and 1-D electrolyzer performance modeling in Python
- Managed daily laboratory operations including: performing safety inspections; developing SOPs for new and safe experimental processes; repairing equipment; keeping an updated chemical and material inventory; purchasing and material budgeting; training, onboarding, and mentoring new students; and organizing group schedules, responsibilities, and events
- Taught and planned weekly electrochemistry lectures for younger graduate students

Argonne National Laboratory, Lemont, IL *May 2018-August 2018*
Science Undergraduate Laboratory Internship (SULI) Summer Researcher
- Utilized existing programs and developed original Python code to model vibrational energies for 60 combustion-related molecules using vibrational perturbation theory
- Generated predictive values for thermodynamic properties of combustion-related species using analytical and direct-count computational approaches

Brushett Lab at Massachusetts Institute of Technology, Cambridge, MA *June 2017-August 2017*
Summer Research Affiliate
- Electrochemically enhanced and characterized carbon electrode microstructures to improve the performance of aqueous and nonaqueous redox flow batteries
- Studied impedance and battery performance using electrochemical software

Willis Laboratory at University of Connecticut, Storrs, CT *August 2017-August 2019*
Undergraduate Researcher
- Developed a MATLAB model to predict signal output of a multi-component array of vapor sensors
- Fabricated gold nanoparticle semiconductor electrodes for sensitive and selective chemical vapor sensors
- Designed prototypes for fluid flow tables to enable efficient spatial atomic layer deposition

Mustain Laboratory at University of Connecticut, Storrs, CT *January 2017-May 2017*
Undergraduate Researcher
- Synthesized metal oxide anodes and assembled Li-ion batteries to improve energy density and cycle life
- Conducted and analyzed capacity retention and impedance tests

Skills and Certifications

Technical Skills: MATLAB, Python, Linux, electrochemical device testing and characterization, Aspen, SolidWorks, 1-D electrochemical modeling, chemical vapor deposition, ion chromatography, SEM
Languages: Conversational French
Certifications: NCEES Engineer-In-Training

Alexandra Oliveira

Awards and Fellowships

NSF Graduate Research Fellow *April 2020-Present*
University of Delaware Collins Fellow *January 2020-August 2020*
University of Delaware Saurabh A. Palkar Graduate Award for Mentoring Fellowship *May 2022*

Teaching, Volunteer, and Leadership

University of Delaware Dept. of Chemical Engineering, Newark, DE *February 2021-December 2021*
Graduate Teaching Assistant
Colburn Club, University of Delaware, Newark, DE *September 2021-Present*
Outreach Committee Lead

- Tutored students in algebra and organized science demos at Shue-Medill Middle School

University of Connecticut Chem-E-Car Team, Storrs, CT *January 2016-May 2019*
President, Member

- Designed a car powered by a chemical reactor and competed regionally and nationally
- Mentored a six-member team to construct a homemade aluminum air battery

American Institute of Chemical Engineers, UConn Chapter, Storrs, CT *January 2016-May 2019*
President, Vice President, Member

Selected Publications

Oliveira, A.M.; Beswick, R.R.; Yan, Y. A Green Hydrogen Economy for a Renewable Energy Society. *Current Opinions in Chemical Engineering*. **2021**, *33*, 100701.

Beswick, R.R.*; **Oliveira, A.M.***; Yan, Y. Does the Green Hydrogen Economy Have a Water Problem? *ACS Energy Lett.* **2021**, *6*(9), 3167-3169.

Oliveira, A.M.; Beswick, R.R.; Yan, Y. Trends in the Recognition of Women in Electrochemistry. *J. Electrochem. Soc.* **2022**, *169*(2) 023508.

Xiao, J.; **Oliveira, A.M.**; Wang, L.; Zhao, Y.; Wang, T.; Wang, J.; Setzler, B.P.; Yan, Y. Water-Fed Hydroxide Exchange Membrane Electrolyzer Enabled by a Fluoride-Incorporated Nickel-Iron Oxyhydroxide Oxygen Evolution Electrode. *ACS Catal.* **2021**, *11*, 264-270.

Forner-Cuenca, A.; Penn, E.E.; **Oliveira, A.M.**; Brushett, F.R. Exploring the Role of Electrode Microstructure on the Performance of Non-Aqueous Redox Flow Batteries. *J. Electrochem. Soc*. **2019**, *166*, A2230-A2241.

Palmieri, A.; Yazdani, S.; Kashfi-Sadabad, R.; Karakalos, S.G.; Ng, B.; **Oliveira, A.**; Peng, X.; Pettes, M.T.; Mustain, W.E. "Improved Capacity Retention of Metal Oxide Anodes in Li-Ion Batteries: Increasing Intraparticle Electronic Conductivity through Na Inclusion in Mn_3O_4", *ChemElectroChem.* **2018**, *5*(15), 2059-2063.

Selected Presentations

Alexandra M. Oliveira, Brian P. Setzler, Yushan Yan, "Anode-Fed Anion Exchange Membrane Electrolyzers for Hydrogen Generation Tolerant to Anion Contaminants." ECS Meeting Abstracts, 2022, 1679.

Alexandra Oliveira, Antoni Forner-Cuenca, Fikile Brushett, "Towards Advanced Porous Carbon Electrodes for Redox Flow Batteries." Poster presentation at the 2017 Annual Meeting of the American Institute of Chemical Engineers. October 30, 2017, Minneapolis, MN.

- 3^{rd} place Harry West Student Poster Award, sponsored by Honeywell, Inc.
- 3^{rd} place award for division three of Fuels, Petrochemicals, and Energy

Alexandra Oliveira, Savanna Dautle, Lawrence Harding, Bryan Changala, John Stanton, Eric Phipps, Branko Ruscic, David Bross, "Generation of Accurate Anharmonic Partition Functions Using Vibrational Perturbation Theory." Poster presentation at the Argonne Learning on the Lawn Poster Session. August 1, 2018.

BRIAN PAUL

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Education

University of Delaware, Newark DE — Expected 2024
PhD Candidate, Chemical & Biomolecular Engineering

University of California, Irvine — June 2019
B.S., Chemical Engineering — GPA: 3.75/4.0
B.S., Materials Science & Engineering
Graduated *Cum Laude* · Tau Beta Pi & Omega Chi Epsilon Engineering Honor Societies

Irvine Valley College — May 2015
A.A., Social & Behavioral Science — GPA: 3.95/4.0
Graduated *Magna Cum Laude* · Earned Associate Degree during high school

Research Experience

Graduate Researcher, University of Delaware — Sept 2019 – Present
Advisors: Dr. Norman Wagner, Dr. Eric Furst, Dr. Abraham Lenhoff, and Dr. Susana Teixeira

Guest Researcher, NIST Center for Neutron Research, Gaithersburg, MD — Jan 2022 – Present

- Investigating the effects of high pressure on protein clustering in the presence of precipitants via small-angle x-ray scattering (SAXS), dynamic light scattering, size-exclusion chromatography, and spectroscopy
- Characterized local crystalline ordering within salted-out protein dense phases via small-angle scattering
- Collaborating with NCNR beamline scientists to design and construct novel instrument for simultaneous small-angle neutron scattering (SANS) and diffusing wave spectroscopy (DWS) under high pressure

Undergraduate Researcher, UC Irvine, Colloid Science Laboratory (Mohraz Group) — Sept 2017 – June 2019
Advisor: Dr. Ali Mohraz

- Demonstrated potential for bijel production from novel fluid systems to simplify scaffold production
- Designed Stober process to synthesize silica particles 80-500 nanometer in diameter

Undergraduate Research Assistant, UC Irvine, Ceramics Laboratory (Mecartney Group) — Sept 2016 – Mar 2017
Advisor: Dr. Martha Mecartney

- Polished ceramic samples for SEM and XRD analysis; analyzed grain sizes via ImageJ

Selected Presentations

1. **B. Paul,** N.J. Wagner, E.M. Furst, A.M. Lenhoff, S.C.M. Teixeira. "Structural Investigation of Salt-Induced Local Ordering in Protein Dense Phases." 95th ACS Colloid and Surface Science Symposium, June 14 – 16, 2021, virtual (oral presentation.)
2. **B. Paul,** N.J. Wagner, E.M. Furst, A.M. Lenhoff, S.C.M. Teixeira. "Ovalbumin Dense Phase Formation in Concentrated Electrolyte Solutions." Neutrons and Food 6, May 16 – 18, 2022, virtual (oral presentation.)
3. **B. Paul,** N.J. Wagner, E.M. Furst, A.M. Lenhoff, S.C.M. Teixeira. "Crystal, Liquid, or Gel: A Thermodynamic Framework for Phase Behavior in Dilute Protein Solutions with Increasing Salt Concentration." 11th American Conference on Neutron Scattering, June 5 – 9, 2022, Boulder CO (poster presentation.)

Skills

Characterization: Circular dichroism (CD), small-angle neutron scattering (SANS), small-angle x-ray scattering (SAXS), static/dynamic light scattering (SLS/DLS), bulk rheology, diffusing wave spectroscopy (DWS) microrheology, optical microscopy, size exclusion chromatography (SEC)
Computational: Aspen, AutoCAD, BioXTAS RAW, Cura (3D printing), IGOR, ImageJ, MATLAB, Minitab, Origin, Pro/II, PyMOL, SasView, SimCentral, Simulink, SolidWorks, TRIOS

Publications

1. **Paul, B.;** Furst, E.M.; Lenhoff, A.M.; Teixeira, S.C.M.; Wagner, N.J. Influence of high hydrostatic pressure on salt-induced protein clustering. 2023 (In preparation)
2. Ching, H.; Thorson, T.J.; **Paul, B.**; Mohraz, A. Rapid production of bicontinuous microporous materials using intrinsically polymerizable bijels. *Materials Advances* 2021, 2, 5067-5075, 2021.

Teaching Experience

Graduate Teaching Assistant (double assignment), University of Delaware Feb 2021 – June 2021

- Held biweekly office hours for 70 CBE sophomores in classical thermodynamics; managed six graders
- Developed course design project in ASPEN PLUS; delivered two 90-minute tutorial lectures

Guest Instructor, Center for High Resolution Neutron Scattering, Gaithersburg, MD Feb 2021, Oct 2022

- Assisted with BioSANS sessions for 26th, 27th Schools on Neutron Scattering & Reflectometry
- Guided groups of 3-4 graduate students in SANS data reduction, fitting, and analysis

Industry Experience

Engineering Prototyping Lab Intern, UCI Applied Innovation, Irvine, CA June 2018 – June 2019

- Trained engineers on prototyping equipment and assisted lab users; wrote optical microscope SOP

Chemical Process Software Test Intern, Schneider-Electric, Lake Forest, CA June 2017 – Sept 2017

- Beta tested SimCentral 1.8; logged defects and developed an 8-step checklist to improve existing test cases

Chemical Engineering R&D Intern, Schneider-Electric, Lake Forest, CA June 2016 – Sept 2016

- Developed thermodynamic model for asphaltene deposition in deep sea oil pipes

Selected Awards & Grants

- MRS Student Travel Grant, American Conference on Neutron Scattering June 2022
- Chancellor's Award of Distinction, University of California Irvine June 2019
- Summer Undergraduate Research Fellowship June 2018

Leadership Experience

President, American Chemical Society Biotechnology Division Sept 2021 – Present

- Lead monthly meetings to plan upcoming Chapter programming
- Expanded Mid-Atlantic Chapter to include two additional institutions; initiated new Bay Area Chapter
- Founded national mentorship program to connect graduate students with industry mentors

Recruiting/Communications Lead, American Chemical Society Biotechnology Division Sept 2019 –Aug 2021

- Maintained active member and industry contact list; organized inter-regional forum on D&I in academia

Vice President of External Affairs, American Institute of Chemical Engineers at UCI Apr 2018 – June 2019

- Organized networking & recruiting events with local companies for AIChE members
- Expanded Chapter network and represented AIChE at UCI in all external communications

Regional Conference Sponsorship Chair, American Institute of Chemical Engineers at UCI Oct 2017 – Apr 2018

- Obtained $4000 in corporate sponsorship; organized CBE Career Fair for 250 attendees

Volunteer Experience

Elected Co-Chair, 2024 Gordon Research Seminar on Colloids, Macromolecules, and Polyelectrolyte Solutions
Peer Mentor, UD CBE EmPOWER , Newark, DE Aug 2021 - Present
Outreach Coordinator, Colburn Club, Newark, DE Sept 2019 – Aug 2021
Undergraduate Volunteer, ASM Materials Camp, Irvine, CA June 2018

Esun Selvam

PhD Candidate | Chemical & Biomolecular Engineering | University of Delaware

Email: esuns@udel.edu
Phone: 302-763-2764
LinkedIn: in/esunselvam

EDUCATION

University of Delaware (UD), Newark, DE **2019 - Present**
Ph.D. in Chemical & Biomolecular Engineering

National Institute of Technology-Trichy (NITT), Tiruchirappalli, India. **2015 - 2019**
B. Tech. (Honors) in Chemical Engineering

RESEARCH EXPERIENCE

UD | Graduate Research Assistant | Prof. Dionisios G. Vlachos **2019 - Present**

- Developed heterogeneous catalysts for the rapid depolymerization of Polyethylene Terephthalate (PET) waste to its monomer using microwave heating, achieving high productivity of the process.[1]
- Designed and developed a single-pot microwave assisted strategy to upcycle polyolefin plastic waste selectively to medium-sized olefins in seconds at modest temperatures with unprecedented selectivity to olefins.[3]
- Investigating the influence of different acid sites of mesoporous aluminosilicate catalysts' on the microwave-assisted deconstruction of polyolefins to medium-sized olefins.
- Research Exchange | **University of Zaragoza, Spain**
  - Performed microwave-assisted plastic pyrolysis and propane dehydrogenation experiments with heterogeneous catalysts using a high-efficiency microwave reactor designed by the ITACA institute at Valencia in collaboration with the Santamaria Group at Zaragoza.

Monash University, Melbourne, Australia | Research Assistant | Prof. Akshat Tanksale **May - August, 2018**

- Investigated the effect of different solid-acid supports on the synthesis of Oxymethylene Ethers via methanol mediated CO_x hydrogenation

Indian Institute of Technology – Madras (IITM), Chennai, India | Research Assistant **2016 - 2017**

- **Prof. R. Vinu** | Department of Chemical Engineering **June - August, 2017**
  Researched hydro-pyrolysis of woody biomass using porous Alumina and Zeolite-based catalysts
- **Prof. R. Sarathi** | Department of Electrical Engineering **May - July, 2017**
  Studied the synthesis and characterization of nanostructured Alumina and Titania by wire-explosion method
- **Prof. P. Selvam** | National Centre for Catalysis Research **December 2016 - May 2017**
  Worked on the synthesis, characterization and catalytic properties of Hierarchical- and Nano-Zeolites

NITT | Undergraduate Final Year Project | Prof. T.K. Radhakrishnan **2018 - 2019**

- Designed a chemical process plant for the synthesis of Dimethylformamide (DMF)

TECHNICAL SKILLS

- Microwave Chemistry & Instrumentation
- Thermometry & Sensing in Intense Electromagnetic Environments
- Catalyst Synthesis (Supported catalysts, Metal Oxides, microporous and hierarchical Zeolites)
- Liquid & Gas Chromatography
- Mass Spectrometry
- Fourier Transform Infrared Spectroscopy (Transmission and DRIFTS)
- Scanning Electron Microscopy + EDX
- Transmission Electron Microscopy
- X-ray Diffraction
- Small-Angle X-Ray Scattering
- Nuclear Magnetic Resonance Spectroscopy
- Raman Spectroscopy
- UV-Vis Spectroscopy
- Thermal Analysis (TGA, DSC, TPO)
- High Pressure & Slurry Reactors

LEADERSHIP EXPERIENCE

- **Mentor**, EmPOWER, University of Delaware, a graduate student organization that serves as a low-barrier peer support group to promote mental health in graduate school.
- **Captain**, NIT-Trichy Swimming Team, Tiruchirappalli, India, 2018-19.
- **Treasurer**, Sports Contingent, NIT-Trichy, Tiruchirappalli, India, 2018-19.
- **Treasurer**, SPORTSFETE-18, The Annual Inter-Departmental Sports Fest, NIT-Trichy, 2018-19.
- **Organiser,** FESTEMBER, The Annual Inter-College Cultural Festival, NIT-Trichy, 2016-18.
- **Quality Assurance Co-ordinator,** PRAGYAN, an ISO 9001 & 20121 certified "*Annual International Techno-Management Organization*" of the NIT-Trichy.

TEACHING EXPERIENCE

UD | Graduate Teaching Assistant

- CHEG 445 – Senior Lab (Bio-diesel)
- CHEG 112 – Introduction to Chemical Engineering

EXTRA-CURRICULAR ACTIVITIES

- School- and College-level Swimmer – (Won medals at inter-school and Inter-university/Inter-college level).
- Soccer and Cricket player at the Intra-college level.
- Former member of *Illuminate*, which is a government certified Charitable Trust which aims at developing the lives of children of the marginalized communities.

SELECTED PRESENTATIONS

UCRA 2022 | Leamington Spa, United Kingdom | Oral Presentation

- "Electrified depolymerization of PET over heterogeneous ZnO catalysts"

NAM 2022 | Manhattan, NY | Oral Presentation

- "Microwave-assisted depolymerization of PET over heterogeneous ZnO catalyst"

23rd National Symposium on Catalysis | Bengaluru, India | Poster Presentation

- "Nanozeolite with brain-coral morphology: A self-organized nanostructured material that mimics nature"

PEER-REVIEWED PUBLICATIONS

1. **E. Selvam**, Y. Luo, M. Ierapetritou, R.F. Lobo and D.G. Vlachos, "*Electrified depolymerization of PET over heterogeneous catalysts"*, Catal. Today *(Under review – UCRA2 Special Issue).*
2. Y. Luo, **E. Selvam**, D.G. Vlachos and M. Ierapetritou, *"Economic and Environmental Benefits of Modular Microwave-assisted PET Depolymerization",* ACS Sustain. Chem. Eng. *(Under review).*
3. **E. Selvam**, P.A. Kots, B. Hernandez, A. Malhotra, W. Chen, J.M. Catala-Civera, J. Santamaria, M. Ierapetritou and D.G. Vlachos, *"Plastic waste upgrade to olefins via mild slurry microwave pyrolysis over solid acids*", Chem. Eng. J., 454 (2023) 140332.
4. **E. Selvam**, R.K. Parsapur, C. Hernandez-Tamargo, N. de Leeuw and P. Selvam, *"Nanostructured zeolite with brain-coral morphology and tailored acidity: a self-organized hierarchical porous material with MFI topology"* CrystEngComm, 22 (2020) 6275-6286.
5. P. Ranjan, **E. Selvam**, R. Jayaganthan, H. Suematsu and R. Sarathi, *"Thermodynamic Modelling and Characterisation of Titania Nanoparticles Produced by Wire Explosion Process", Mater. Today: Proc.,* 5 (2018) 17304-17311.
6. P. Ranjan, R. Sarathi, **E. Selvam**, H. Suematsu , P. Selvam and R. Jayaganthan, *"Synthesis of γ-Alumina Nanoparticles by Wire-Explosion Process: Characterisation and Formation Mechanism",* Proc. Int. Conf. on High Voltage Engineering and Power Systems*,* Bali, Oct 2-5, 2017, pp. 301-306.

SANJANA SRINIVAS |
UNIVERSITY OF DELAWARE
Ph.: +13028281160 E-mail: sanjana@udel.edu

EDUCATION

- **UNIVERSITY OF DELAWARE** AUG'19 - PRESENT
  PH.D. IN CHEMICAL ENGINEERING | GPA: 3.96/4
  - **Thesis**: Rational design of supported atomically dispersed transition metal catalysts for dehydrogenation chemistry
- **INDIAN INSTITUTE OF TECHNOLOGY, MADRAS** AUG'15 - MAY'19
  B.TECH. IN CHEMICAL ENGINEERING | GPA: 9.19/10
  - **Thesis**: Conductivity studies on single crystal double perovskites for water splitting applications

HONORS AND AWARDS

- Awarded the **Saurabh A. Palkar Graduate Award** for mentoring fellowship by the University of Delaware 2022
- Awarded the best **Communication Award** at the 18^{th} ICTAC conference, Lyon, France 2022
- Awarded the **Morton and Donna Collins Chemical Engineering Fellowship** by the University of Delaware 2020
- Awarded the **JASSO Scholarship** by the Government of Japan for research at the University of Tokyo 2018
- **National winner** of the **Citi Women Leader Award**, India 2018

PUBLICATIONS

- Dong, Q.; Yao, Y.; Cheng, S.; Alexopoulos, K.; Gao, J.; **Srinivas, S.**; Wang, Y.; Pei, Y.; Zheng, C.; Brozena, A.; Wang, X.; Dai, J.; Zhao, H.; Zheng, W.; Toraman, H.; Lin, Z.; Yang, B.; Ju, Y.; Vlachos, D.; Liu, D.; Hu, L. Programmable Heating and Quenching for Efficient Thermochemical Synthesis, Nature, 2022
- Kewei, Y.; **Srinivas, S.**; Wang, C.; Chen, W.; Ma, L.; Ehlrich, S.; Marinkovic, N.; Kumar, P.; Stach, E.; Caratzoulas, S.; Zheng, W.; Vlachos, D. High-Temperature Pretreatment Effect on Co/SiO_2 Active Sites and Ethane Dehydrogenation, ACS Catalysis, 2022
- **Srinivas, S.**; Vlachos, D. Tuning at the subnanometer scale, Nature Catalysis, 2022, News and Views article (on invitation)
- **Srinivas, S.**; Vlachos, D.; Caratzoulas, S. Spin-Crossing in Heterogeneous Ethane Dehydrogenation By Atomically Dispersed Co/SiO_2, Chem Catalysis (Under revision)
- Wu, J.; **Srinivas, S.**; Caratzoulas, S.; Li, B.; Hawkins, J.; Scott, S. Direct Catalytic Synthesis of N-substituted Azacycles from Cyclic Ethers, (under preparation)
- **Srinivas, S.**; Srivastava, K.; Vlachos, D. Effect of heterogeneity of silica supported Co(II) sites on small alkane dehydrogenation kinetics, (under preparation)

CONFERENCE PRESENTATIONS AND INVITED LECTURES

- "Effect of heterogeneity of silica supported Co(II) sites on small alkane dehydrogenation kinetics", American Institute of Chemical Engineers Annual Meeting, Phoenix, AZ, USA, November 17, 2022
- "Spin-crossing in heterogeneous catalysis by atomically dispersed transition metals. An example: Ethane dehydrogenation by Co/SiO_2", International Conference on Theoretical Aspects of Catalysis (ICTAC), Lyon, France, June 16, 2022
- "Spin-Crossing in heterogeneous catalysis By atomically dispersed transition metals: Ethane Dehydrogenation By Co/SiO_2", 27^{th} North American Catalysis Society Meeting, New York City, USA, May 27, 2022
- "Mechanistic understanding of the effect of active site size in the dehydrogenation of ethane on highly dispersed Co/SiO_2 catalyst", American Institute of Chemical Engineers Annual Meeting, Boston, MA, USA, November 11, 2021
- "Theoretical insights into ethane dehydrogenation on mononuclear and dinuclear Co/SiO_2 catalyst", Invited Student speaker, Catalysis Club of Philadelphia Monthly Meeting, March 24, 2022

Academic Experience

- **Rational design of supported atomically dispersed transition metal catalysts for dehydrogenation chemistry** Jan'20 - Present
  (Advisor: Prof. Dionisios Vlachos, Vlachos Research Group, University of Delaware)
  - Developed the reaction mechanism and electronic descriptors to predict small alkane dehydrogenation activity on Co/SiO_2 of different nuclearity using Density Functional Theory(DFT) and microkinetic modelling
  - Used the insights to predict activity on related 3d metal catalysts and introduced the Fukui index descriptor to predict suitable dopants that enhance activity
  - Predicted the effect of support heterogeneity on the dehydrogenation activity using DFT and ab-initio molecular dynamics
  - Investigated the kinetic stability of subnanometer Pt clusters in CHA and Sn-CHA frameworks (efficient catalyst for small alkane dehydrogenation) using DFT and ab-initio molecular dynamics. Developing -Machine Learning frameworks to shorten simulation times

- **Conductivity Studies for Double Perovskites** Aug'18 - May'19
  (Guide: Dr. Aravind Kumar Chandiran, Solar Energy Research Group, IIT Madras)
  - Optimized the solvothermal synthesis procedure to make single crystals of the double perovskite: $Cs_2AgBiCl_6$
  - Investigated the conduction mechanism in the single crystal using Temperature dependent Impedance Spectroscopy, XPS and in-situ XRD + Linear Sweep Voltammetry

- **Metal Deposition on polymer substrates using Supercritical Fluid Deposition** May'18 - Jul'18
  (Guide: Dr. Yukihiro Shimogaki, Shimogaki-Momose Lab, University of Tokyo)
  - Optimized the oxygen annealing polymer pretreatment protocol and showed successful deposition of Pd and Cu films on the polymer in hot wall reactors for waveguide applications.
  - Analysed the morphology and thickness of the films using SEM and AFM

- **CZTS as absorber in p-DSSC (Dye Sensitised Solar Cells) type architecture** Apr'17 - May'18
  (Guide:Dr. Aravind Kumar Chandiran, Solar Energy Research Group, IIT Madras)
  - Optimized the deposition protocol of CZTS films on NiO, which was chosen as a photocathode in p-DSSCs to replace conventional dyes that have poor adhesion to NiO
  - Studied the morphology of CZTS thin films using SEM, film and device stability in different redox species ($\mathbf{I^-/I_3^-}$, $\mathbf{Co^{3+}/Co^{2+}}$ and polysulphides) using XRD, excited state lifetimes using Time Resolved Single Photon Counting and charge transfer mechanism using Impedance Spectroscopy

Skills

- **Simulation and Theory techniques:** Density Functional Theory (DFT), Time Dependent DFT, XANES, chemical kinetic modeling, Molecular Dynamics, Thermodynamic Integration, Metadynamics
- **Programming and Software:** Python, R, MATLAB, Simulink, ImageJ, VMD, PyMol, Gaussian, VASP, Amber, GAMESS, ADF, CP2K, VESTA, Multiwfn, FDMNES, FEFF
- **Synthesis:** Supercritical Fluid Deposition, Chemical Vapour Deposition, Spin Coater, Hydrothermal Reactor Synthesis
- **Characterisation:** SEM+EDAX, XPS, Optical Microscope, X-Ray Diffraction, TGA, Cyclic Voltammetry, Chrono-Amperometry, UV-Vis, Impedance Spectroscopy, Time Resolved Single Photon Counting

Teaching and Mentorship

2021-Present	Mentored 2 undergraduate researchers at the University of Delaware: Kaveri Srivastava (2021-2022) and Robert Oratorio (2022-Present)
2022-Present	Lead Mentor at EmPOWER, a graduate student organization that serves as a low-barrier peer-support group to promote mental health in graduate school
2020-2022	Student Mentor at EmPOWER
2021	Teaching assistant for CHEG810 Graduate Molecular Thermodynamics at UD Chemical Engineering with Prof. Norman Wagner and Prof. Eric Furst

Huayu Tian

302-357-2610| hytian@udel.edu | https://www.linkedin.com/in/huayu-tian/

EDUCATION

University of Delaware, DE, United States Sep 2019 – Present
Ph.D. Candidate in Chemical and Biomolecular Engineering, GPA: 3.64/4.00
Sichuan University, Sichuan, China Sep 2015 – June 2019
B.Eng. in Chemical Engineering and Technology, GPA: 3.80/4.00

RESEARCH EXPERIENCE

Graduate Research Assistant, University of Delaware Newark, DE
Thesis Advisor: Dr. Marianthi Ierapetritou Jan 2020 – Present

- Reduced computational cost of simulation optimization problems by developing surrogate-based feasibility analysis and optimization frameworks using machine learning models and adaptive sampling strategies
- Improved quality control under uncertainty for solid-based continuous pharmaceutical manufacturing by developing uncertainty quantification methods for residence time distribution-based disturbance tracking

Undergraduate Researcher, Sichuan University Sichuan, China
Intelligent Process and Advanced Control Technology Research Center March 2018 – June 2019
Research Advisor: Dr. Xu Ji

- Employed neural networks optimized with genetic algorithms to diagnose faults for the Tennessee Eastman process

Membrane Science and Functional Materials Group March 2017 – May 2018
Research Advisor: Dr. Liangyin Chu

- Fabricated magnetic microswimmers with hollow helical structures per microfluidic template synthesis, dicing treatment, and biosilicification process

PUBLICATIONS

- **Tian, H.**, Ierapetritou, M. A Surrogate-Based Framework for Feasibility Analysis and Optimization of Expensive Simulations. (In preparation)
- **Tian, H.**, Bhalode, P., Razavi, S., Koolivand, A., Muzzio, F., Ierapetritou, M. Characterization and Propagation of RTD Uncertainty for Continuous Powder Blending Processes. International Journal of Pharmaceutics, 2022. 628: p. 122326.
- Bhalode, P., **Tian, H.**, Gupta, S., Razavi, S., Roman-Ospino, A., Talebian, S., Singh, R., Scicolone, J., Muzzio, F., Ierapetritou, M. Using Residence Time Distribution in Pharmaceutical Solid Dose Manufacturing – A Critical Review. International Journal of Pharmaceutics, 2021. 610: p. 121248.
- Tang, M., Wang, W., Li, Z., Liu, Z., Guo, Z., **Tian, H.**, Liu, Z., Ju, X., Xie, R., Chu, L. Controllable Microfluidic Fabrication of Magnetic Hybrid Microswimmers with Hollow Helical Structures. Industrial & Engineering Chemistry Research, 2018. 57(29): p. 9430

CONFERENCE PRESENTATIONS

- **Tian, H.** and Ierapetritou, M. "A Surrogate-Based Framework for Feasibility Analysis and Optimization of Expensive Simulations", **Oral Presentation** #624c, AIChE Annual Meeting, Phoenix, AZ, November 2022.
- **Tian, H.**, Bhalode, P., Razavi, S., Roman-Ospino, A., Muzzio, F., Ierapetritou, M., "Development of RTD-Based Flowsheet Modeling Including Process Uncertainty for Continuous Solid-Based Drug Manufacturing", **Oral Presentation** #308c, AIChE Annual Meeting, Boston, MA, November 2021.

TEACHING EXPERIENCE

Graduate Teaching Assistant, University of Delaware Newark, DE

- CHEG 341: Fluid Mechanics Fall 2021
- MATH 305: Applied Math for Engineers Spring 2021
  - Created MATLAB tutorial videos with 900+ views

SKILLS

Programming Languages: MATLAB, Python, GAMS, gPROMS, C++
Software & Tools: MS Office, Minitab, AutoCAD, Origin, Aspen Plus, Simulink, Active Presenter

Brandon C. Vance

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221 Academy St., ISE Building Suite 165, Newark, DE 19716

Education

University of Delaware **August 2019 – Present (Anticipated June 2023)**
Ph.D. Chemical Engineering (GPA: 3.36) Advisor: Prof. Dionisios G. Vlachos
Iowa State University **August 2015 – May 2019**
B.S. Chemical Engineering (GPA: 3.49)

Experience

NSF Graduate Research Fellow **Jan. 2020 – May 2023**
University of Delaware, USA
Investigating the Mechanism of Polyolefin Hydroconversion
Catalyst Development and Design for Polyolefin Hydroconversion
Extension of Hydroconversion Chemistries Beyond Polyolefin Feedstocks

Visiting Scholar **Jun. 2019 – Jul. 2019**
Prof. Qiang Lu, North China Electric Power University, China
Catalytic Pyrolysis of Biomass to Hydroxylactones

NASA Undergraduate Research Fellow **Sept. 2017 – May 2019**
Prof. Jean-Philippe Tessonnier, Iowa State University, USA
Metal-Support Interactions in Noble Metal Catalysts
Impact of Thermal Gradients on Catalyst Selectivity and Deactivation in CO_2 Methanation

Ronald E. McNair Scholar **Aug. 2017 – May 2019**
Dr. Thelma L. Harding, Iowa State University, USA

Refereed Publications

(1) Petersen, E.M.; Rao, R.G.; **Vance, B.C.**; Tessonnier, J.-P. SiO2/SiC Supports with Tailored Thermal Conductivity to Reveal the Effect of Surface Temperature on Ru-Catalyzed CO2 Methanation. *Appl. Catal. B Environ.* **2021**, *286*, 119904.
(2) Liu, S.; Kots*, P.A., Kots*; **Vance, B.C.***; Danielson, A.; Vlachos, D.G. Plastic Waste to Fuels by Hydrocracking at Mild Conditions. *Sci. Adv.* **2021**, *7* (17), eabf8283. *co-first author
(3) Kots, P.A.; Liu, S.; **Vance, B. C.**; Wang, C.; Sheehan, J.D.; Vlachos, D.G. Polypropylene Plastic Waste Conversion to Lubricants over Ru/TiO2Catalysts. *ACS Catal.* **2021**, *11*, 8104–8115.
(4) **Vance, B.C.**; Kots, P.A.; Wang, C.; Hinton, Z.R.; Quinn, C.M.; Epps, T.H.; Korley, L.T.J.; Vlachos, D.G. Single Pot Catalyst Strategy to Branched Products via Adhesive Isomerization and Hydrocracking of Polyethylene over Platinum Tungstated Zirconia. *Appl. Catal. B Environ.* **2021**, *299*, 120483.
(5) Wang, C.; Xie, T.; Kots, P.A.; **Vance, B.C.**; Yu, K.; Kumar, P.; Fu, J.; Liu, S.; Tsilomelekis, G.; Stach, E.A.; Zheng, W.; Vlachos, D.G. Polyethylene Hydrogenolysis at Mild Conditions over Ruthenium on Tungstated Zirconia. *JACS Au* **2021**, *1* (9), 1422–1434.
(6) Kots, P.A.*; **Vance, B.C.***; Vlachos, D.G. Polyolefin Plastic Waste Hydroconversion to Fuels, Lubricants, and Waxes: a Comparative Study. *React. Chem. Eng.* **2022**, *7*, 41-54. *co-first author
(7) Hinton, Z.R.; Kots, P.A.; Soukaseum, M.; **Vance, B.C.**; Vlachos, D.G.; Epps T.H.; Korley, L.T.J. Antioxidant-Induced Catalyst Transformations in the Hydrocracking of Polyethylene Waste. *Green Chem.* **2022**.
(8) Wang, C.; Yu, K.; Sheludko, B.; Xie, T.; Kots, P.A.; **Vance, B.C.**; Kumar, P.; Stach, E.A.; Zheng, W.; Vlachos, D.G. A General Strategy and a Consolidated Mechansims for Low-methane Hydrogenolysis of Polyethylene over Ruthenium. *Appl. Catal. B Environ.* **2022**, *319*, 121899.
(9) Kots, P.A.; Xie, J.; **Vance, B.C.**; Quinn, C.M.; Dorneles de Mello, M.; Boscoboinik, J.A.; Wang, C.; Kumar, P.; Stach, E.A; Marinkovic, N.S.; Ma, L.; Ehrlich S.N.; Vlachos, D.G. Electronic Modulation of Metal-Support Interactions Improves Polypropylene Hydrogenolysis Over Ruthenium Catalysts. *Nat. Comm.* **2022**, *131*, 1-11.
(10) **Vance, B.C.**; Kots, P.A.; Wang, C.; Granite, J.E.; Vlachos, D.G. Ni/SiO_2 Catalysts for Polyolefin Deconstruction via the Divergent Hydrogenolysis. *Appl. Catal. B Environ.* **2022**, *322*, 122138.
(11) **Vance, B.C.**; Najmi, S.; Kots, P.A.; Wang, C.; Granite, J.E.; Oberhausen, C.; Jeon, S.; Stach, E.A.; Vlachos, D.G. Redistribution of Ni in Ni/Al_2O_3 Catalysts for Low-Methane Selectivity in Polyethylene Hydrogenolysis. [**In Preparation**].
(12) **Vance, B.C.**; Najmi, S.; Kots, P.A.; Vlachos, D.G. High-Quality Lubricants from Polystyrene Hydrogenolysis using Ni/SiO_2. [**In Preparation**].

Selected Conference Presentations

(1) **Vance, B.C.**, Petersen E.M., Rao, R.G., Tessonnier, J.-P. Fueling Space Exploration: Engineering Catalysts to Produce Rocket Fuel on Mars, *Posters on the Hill*, Apr. 30, 2019, Washington, D.C., **Poster**.
(2) **Vance, B.C.**; Kots, P.A.; Wang, C.; Vlachos, D.G. Bridging the Gap Between Small Alkane and Polyolefin Hydrocracking, *ACS Fall 2021*, Aug. 22-26, 2021, **Presentation**.

(3) **Vance, B.C.**; Kots, P.A.; Wang, C.; Vlachos, D.G. Bridging the Gap Between Small Alkane and Polyolefin Hydrocracking, *AIChE Annual Meeting*, Nov. 7-19, 2021, **Presentation**.
(4) **Vance, B.C.**; Kots, P.A.; Wang, C.; Hinton, Z.R.; Vlachos, D.G. Mechanistic Insights into the Hydrocracking of Polyolefin Plastics Waste, *ACS Spring 2022*, Mar. 20-24, 2022, **Presentation**.
(5) **Vance, B.C.**; Kots, P.A.; Wang, C.; Vlachos, D.G. Developing a Mechanistic Framework for Polyolefin Hydroconversion, *NAM27*, May 22-27, 2022, **Presentation**.
(6) **Vance, B.C.**; Kots, P.A.; Wang, C.; Vlachos, D.G. Developing a Mechanistic Framework for Polyolefin Hydroconversion, *Catalysis Club of Philadelphia Summer Symposium*, June 8, 2022, **Poster**.
(7) **Vance, B.C.**; Kots, P.A.; Wang, C.; Vlachos, D.G. Developing a Mechanistic Framework for Polyolefin Hydroconversion, *ACS Fall 2022*, Aug. 21-25, **Presentation**.
(8) **Vance, B.C.**; Kots, P.A.; Vlachos, D.G. Polyolefin Upcycling over Earth-Abundant Catalysts, *AIChE Annual Meeting*, Nov 13-18, 2022, **Presentation.**

Honors, Awards, and Fellowships

Catalysis Club of Philadelphia Best Presentation **June 2022**
Recognition for best poster presentation at the CCP's Summer Symposium

NAM 27 Kokes Travel Award **May 2022**
Received funds to attend the 27th North American Catalysis Society meeting

Theodore A. Koch Travel Award **Apr. 2022**
Received funds from the Catalysis Club of Philadelphia to attend an international conference

ACS CATL Division Travel Award **March 2022**
Received funds to attend the 2022 Spring ACS Conference

NSF Graduate Research Fellowship **Apr. 2020 – Present**
Received a 5-year fellowship from the NSF providing financial support to attend UD

NSF-IRES Visiting Scholar Award **Jun. 2019 – Aug 2019**
Received funds to visit Beijing, China and conduct research for 10-weeks at NCEPU

Engineering Excellence Award **Apr. 2019**
Recognition for outstanding research in STEM from IEEE-USA

NASA Iowa Space Grant Research Fellowship **Aug. 2018 – May 2019**
Received a fellowship from the Iowa Space Grant Consortium from NASA

Mentoring

Jack Granite (Undergraduate Student) **Jun. 2021 – Present**
Optimizing Catalyst Performance in Polyethylene Hydrocracking
Developing High Performance Ni-based Catalysts for Polyethylene Hydrogenolysis
Elucidating the Role of Reaction Products in Polyethylene Hydrocracking
Effect of Metal Identity and Composition in Bimetallic Hydrocracking Catalysts

Christine Oberhausen (Graduate Student) **Jan. 2021 – Present**
Deconstruction of Multilayered Films

Pedro Moura (Graduate Student) **Sept. 2022 – Present**
Solid-Solid Transformations of Oxygenated Polymers

Teaching Experience

Graduate Teaching Assistant **Aug. 2021 – May 2022**
University of Delaware, Chemical and Biomolecular Engineering
Chemical Engineering Kinetics (CHEG 332) Student evaluation score: 4.50/5.00
Heat and Mass Transfer (CHEG 342) Student evaluation score: 4.71/5.00

Undergraduate Teaching Assistant **Aug. 2017 – Dec. 2017**
Iowa State University, Chemistry
General Chemistry I (CHEM 177) Student evaluation score: 4.38/5.00
Laboratory in General Chemistry I (CHM 177L) Student evaluation score: 4.30/5.00

Activities

AIChE graduate student representative, UD CBE **Sept. 2019 – Sept. 2021**
Thrust coordinator, Center for Plastics Innovation **Jan. 2020 – Jan. 2022**
Graduate diversity committee member, UD College of Engineering **Feb. 2020 – May 2021**
EmPOWER mental health peer mentor, UD CBE **Jul. 2020 – Present**
Spring 2021 seminar series organizer, Center for Plastics Innovation **Sept. 2020 – Jun. 2021**
Graduate student-body vice president, UD CBE **Sept. 2021 – Sept. 2022**
Graduate student advisory group, UD College of Engineering **Sept. 2021 – Oct. 2022**

JAYANTH VENKATARAMA REDDY

Newark, Delaware • 4436004086 • jreddy@udel.edu
Date of birth: 01/30/1995

EDUCATION

University of Delaware, Newark, Delaware, USA — **August 2019 - May 2024**
Ph.D in Chemical and Biomolecular Engineering — GPA: 3.83/4.0
Johns Hopkins University, Baltimore, Maryland, USA — **August 2017 - May 2019**
M.S. in Chemical and Biomolecular Engineering — GPA: 3.96/4.0
M. S. Ramaiah Institute of Technology, Bangalore, India — **August 2013 - June 2017**
B.E. in Chemical Engineering — GPA: 9.27/10.0

RESEARCH INTERESTS

Cell culture, Metabolic flux analysis, Metabolic engineering, Mathematical modelling, Modeling N-linked glycosylation

ACADEMIC EXPERIENCE

University of Delaware, Newark, Delaware, USA — **August 2019 - May 2024**

PhD candidate, Co-advised by Prof Marianthi Ierapetritou and Prof Terry Papoutsakis, Chemical and Biomolecular Engineering

- Integrated computational and experimental methods to study the effect of bioreactor pH and Temperature on Chinese Hamster Ovary (CHO) cell metabolism and glycosylation of monoclonal antibodies. Developing models for metabolism and glycosylation to perform model based optimization of bioreactor operation.
- Utilising mathematical models to assist CHO clone selection for further scale up studies.

Johns Hopkins University, Baltimore, Maryland, USA — **August 2017 - June 2019**

Graduate Research Assistant, **Prof Michael J. Betenbaugh, Chemical and Biomolecular Engineering**

- Integrated kinetic and stoichiometric model to predict dynamic metabolic profiles of CHO cell cultures.
- Control of glycolysis in CHO cells and studying its effect on glycosylation by inhibiting certain enzymes in the glycolysis pathways to reduce lactate production.

Graduate Research Assistant, **Prof Marc D. Donohue, Chemical and Biomolecular Engineering**

- Applied solution thermodynamics based models to develop a tool to predict solubilities of media components for cell culture media manufacturing companies.

Lakehead University, Thunder-bay, Ontario, Canada — **June 2016 – September 2016**

Summer Intern, Prof Sudip Rakshit, Biorefining Research Institute

- Production of value added products from crude glycerol (major by-product of the biodiesel industry). Cultured fungi using crude glycerol as a carbon source and converted lipid from the yeast to polyurethane.

Indian Institute of Science, Bangalore, India

Summer Intern, Prof H. N Chanakya, Center for Sustainable Technology — **June 2015 – August 2015**

- Design of biofilm based bioreactor to convert methane in biogas to methanol to be used as a liquid fuel.

Summer Intern, Prof S. Dasappa, Center for Sustainable Technology — **June 2014 – August 2014**

- Modelling of combustion and thermodynamics processes in an IC engine.

PUBLICATIONS

1. Utilisation of microbial oil obtained from crude glycerol for the production of polyol and its subsequent conversion to polyurethane foams, Bioresource technology 235, 309-315, 2017
2. Designing a biofilm based bioreactor to convert methane present in biogas to methanol,IIChE, SCHEMCON 2015

AWARDS

1. Johns Hopkins University ChemBE Master's Essay Scholarship for second-year (2018)
2. "Outstanding graduate student award" from M. S. Ramaiah Institute of Technology in 2017.
3. "Best outgoing chemical engineering student award" from Indian Institute of Chemical Engineers, Bangalore Region in 2017.
4. Mitacs Globalink Internship 2016.

TECHNICAL SKILLS

Laboratory Skills: Algae, Bacteria, Fungi & Mammalian cell culture, ELISA, Western blot, Process modelling & control, YSI analyser, FTIR spectroscopy, SEM, Flow Cytometry, Total Organic Carbon, BET Surface area, HPLC, BioFlo 120 bioreactor
Programming Languages and Softwares: Matlab, Python, C++, C, Autocad, Aspen HYSYS, LaTeX, Bash
Other relevant skills: Flux balance analysis, Kinetic modelling, Parameter estimation, Parallel computing

Piaoping Yang

Chemical and Biomolecular Engineering
University of Delaware, DE 19702, US
Phone: +1-302-747-4169
E-mail: yangpp@udel.edu

EDUCATION

Sep. 2019 ─ Present **Ph.D.** candidate in Chemical Engineering (Supervised by Prof. Dionisios G. Vlachos)
Chemical and Biomolecular Engineering, University of Delaware, US

Sep. 2016 ─ June. 2019 **M.S.** in Chemical Technology (Supervised by Prof. Jinlong Gong)
School of Chemical Engineering & Technology, Tianjin University, China

Sep. 2012 ─ Jun. 2016 **B.S.** in Chemical Engineering & Technology
School of Chemical Engineering, Nanjing Tech University, China

RESEARCH INTERESTS

Density Functional Theory: Biomass upgrading on carbon materials; XANES simulations; Microkinetic modeling; CO_2 reduction on heterogeneous catalysts

SELECTED AWARDS AND HONORS

Apr. 2022 Richard Wool Award for Women in Green Engineering
Nov. 2018 China National Scholarship for Graduate Students
Jul. 2018 Excellent Oral Report of Ph.D. Forum on Chemical Engineering and Resources
Jun. 2016 Excellent Graduate Thesis of Nanjing Tech University
Nov. 2015 China National Scholarship for Encouragement
Aug. 2015 The Third Prize of National College Student Chemical Engineering Design Competition
Nov. 2014 China National Scholarship for Encouragement
Nov. 2013 China National Scholarship for Encouragement

PUBLICATIONS

15. Song Shi§, **Piaoping Yang**§, Chaochao Dun, Weiqing Zheng, Jeffrey J. Urban, Dionisios G. Vlachos*, "Selective hydrogenation via precise hydrogen bond interactions on catalytic scaffolds" ***Nat. Commun.*** under revision

14. Jiahua Zhou,† **Piaoping Yang**,† Pavel Kots, Maximilian Cohen, Matheus de Mello, J. Anibal Boscoboinik, Stavros Caratzoulas,1 Weiqing Zheng* Dionisios G. Vlachos*, "The Role of Oxygen-Containing Functional Groups of Carbon Surfaces" ***Nat. Catal.*** under revision

13. Chen Li, Jiang Li*, Ling Qin, **Piaoping Yang**, and Dionisios G. Vlachos*, "Recent Advances in the Photocatalytic Conversion of Biomass-Derived Furanic Compounds" ***ACS Catal***. 2021, 11, 18, 11336–11359.

12. Chuanye Xiong, Sai Chen, **Piaoping Yang**, Shenjun Zha, Zhi-Jian Zhao*, and Jinlong Gong*, "Structure–performance Relationships for Propane Dehydrogenation over Aluminum Supported Vanadium Oxide" ***ACS Catal***. 2019, 9, 5816-5827.

11. Lulu Li, Zhi-Jian Zhao, Congling Hu, **Piaoping Yang**, Xintong Yuan, Yanan Wang, Lei Zhang, Lyudmila Moskaleva, and Jinlong Gong*, "Tuning Oxygen Vacancies of Oxides for Promoting Electrocatalytic Reduction of Carbon Dioxide" ***ACS Energy Lett***. 2020, 5, 552-558.

10. Dongfang Cheng, Zhi-Jian Zhao, Gong Zhang, **Piaoping Yang**, Lulu Li, Hui Gao, Sihang Liu, Xin Chang, Sai Chen, Tuo Wang, Geoffrey A. Ozin, Zhipan Liu, and Jinlong Gong*, "The Nature of Active Sites for Carbon Dioxide Electroreduction over Oxide-derived Copper Catalysts" ***Nature Commun.*** 2021, 12, 395.

9. **Piaoping Yang**, Zhi-Jian Zhao, Xiaoxia Chang, Rentao, Mu, Shenjun Zha, Gong Zhang, and Jinlong Gong*, "The Functionality of Surface Hydroxy Groups on the Selectivity and Activity of Carbon Dioxide Reduction over Cuprous Oxide in Aqueous Solutions" ***Angew. Chem. Int. Ed.*** 2018, 57, 7724-7728.

8. **Piaoping Yang,** Lulu Li, Zhi-Jian Zhao*, and Jinlong Gong, "Reveal the nature of particle size effect for CO_2 reduction over Pd and Au," ***Chinese J. Catal***. 2021, 42, 817-823.

7. Xiaoxia Chang, Tuo Wang, Zhi-Jian Zhao, **Piaoping Yang**, Jeffrey Greeley, Rentao Mu, Gong Zhang, Zhongmiao Gong, Zhibin Luo, Jun Chen, Yi Cui, Geoffrey A. Ozin, and Jinlong Gong*, "Tuning Cu/Cu_2O Interfaces for Reduction of Carbon Dioxide to Methanol in Aqueous Solutions" ***Angew. Chem. Int. Ed.*** 2018, 57, 15415-15419 **(Cover Story & Hot Article)**.

6. Xiaoxia Chang, Tuo Wang, **Piaoping Yang**, Gong Zhang, and Jinlong Gong*, "The Development of Cocatalysts for Photoelectrochemical CO_2 Reduction", ***Adv. Mater.*** 2019, 31, 1804710

5. Wenjin Zhu, Lei Zhang, **Piaoping Yang**, Congling Hu, Hao Dong, Zhi-Jian Zhao, Rentao Mu, and Jinlong Gong*, "Formation of Enriched Vacancies for Enhanced CO_2 Electrocatalytic Reduction over AuCu Alloys" ***ACS Energy Lett.*** 2018, 3, 2144-2149.

4. Wenjin Zhu, Lei Zhang, **Piaoping Yang**, Congling Hu, Zhibin Luo, Xiaoxia Chang, Zhi-Jian Zhao, and Jinlong Gong*, "Low-Coordinated Edge Sites on Ultrathin Palladium Nanosheets Boost CO_2 Electroreduction Performance" ***Angew. Chem. Int. Ed.*** 2018, 57, 11544-11548 (**Cover Story & Hot Article**)

3. Wenjin Zhu, Lei Zhang, **Piaoping Yang**, Xiaoxia Chang, Hao Dong, Ang Li, Congling Hu, Zhiqi Huang, Zhi-Jian Zhao, and Jinlong Gong*, "Morphological and Compositional Design of Pd-Cu Bimetallic Nanocatalysts with Controllable Product Selectivity towards CO_2 Electroreduction" ***Small*** 2018, 14, 1703314 (**Cover Story**).

2. Ang Li, Tuo Wang, Xiaoxia Chang, Zhi-Jian Zhao, Chengcheng Li, Zhiqi Huang, **Piaoping Yang**, Guangye Zhou, and Jinlong Gong*, "Tunable Syngas Production from Photocatalytic CO_2 Reduction with Mitigated Charge Recombination Driven by Spatially Separated Cocatalysts" ***Chem. Sci.*** 2018, 9, 5334-5340 (**Cover Story & Hot Article**).

1. Hao Dong, Lei Zhang, **Piaoping Yang**, Wenjin Zhu, Zhi-Jian Zhao*, and Jinlong Gong*, "Facet Design Promotes Electroreduction of CO_2 to CO on Palladium Nanocrystals" ***Chem. Eng. Sci.*** 2019, 194, 29-35.

PRESENTATIONS

5 Electrochemical CO_2 Reduction over Cu-based Catalysts, *The 27th North American Catalysis Society Meeting*, May 22-27, 2022 New York, NY **(Oral)**

4 Structure Sensitivity of Catalytic Transfer Hydrogenation of Furfural over Single-Atom Catalysts, *The 27th North American Catalysis Society Meeting*, May 22-27, 2022 New York, NY (Poster)

3 Highly Active Single-Atom Iron Catalysts Towards Catalytic Transfer Hydrogenation of Furfural, *AIChE Annual Meeting*, Nov 7-11, 2021, Boston, MA (**Oral**)

2. The Functionality of Surface Hydroxy Groups on the Selectivity and Activity of Carbon Dioxide Reduction over Cuprous Oxide in Aqueous Solutions, *The 1st Ph.D. Forum on Chemical Engineering and Resources*, July 2018, Beijing, China (**Oral**)

1. Mechanistic Studies of CO_2 Reduction over Cuprous Oxide, *The 13th National Conference of Quantum Chemistry*, Jun 2017, Dalian, China (Poster)

Kewei Yu

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Education

University of Delaware, Newark, DE, U.S. 2019 – Present
Candidate for Doctor of Philosophy
Chemical & Biomolecular Engineering

Nanjing Tech University, Nanjing, Jiangsu, P.R.C. 2015 – 2019
Bachelor of Engineering
Materials Science and Engineering

Research Experience

Graduate Research Assistant 2019 – Present
University of Delaware
Principal Investigator: Dionisios G. Vlachos

- Designed and constructed a programmable Rapid Pulse Joule heating (RPH) reactor for high temperature thermal chemical reactions, including methane dry reforming and propane dehydrogenation
- Investigated the effect of pulse heating on catalyst (PtNi, CuNi) structural evolution using NAP-XPS
- Designed and constructed a Steady-state Isotopic-transient Kinetic Analysis (SSITKA) system. Developed LabView program for integrated instrument control
- Developed a single-site Co/SiO_2 catalyst for ethane non-oxidative dehydrogenation reaction and investigated its high-temperature pretreatment effect through extensive characterizations

Research Intern Summer 2018
University of Alabama
Principal Investigator: Ruigang Wang

- Proposed and conducted LLZO solid state electrolyte synthesis using hydrothermal method to lower the annealing temperature and reduce the lithium loss during heat treatment

Undergraduate Research Assistant 2018 – 2019
Nanjing Tech University
Principal Investigator: Sheng Cui

- Proposed and synthesized carbon/TiCN composite aerogel using Sol-gel method and supercritical drying for Li-S battery cathode material application
- Assembled coin-cell battery for cyclic voltammetry testing

Teaching and Mentoring Experience

Undergraduate Researcher Mentor Summer 2022
Research topic: Structure function relationship of $PtSn/SiO_2$ for propane dehydrogenation reaction

- Formulated research plan for undergraduate student research experience
- Mentored an undergraduate student synthesizing and testing supported metal catalyst for propane dehydrogenation reaction

Graduate Teaching Assistant
CHEG613 Topics for Energy and the Environment Fall 2021

- Graded assignments, news reports and the final project

CHEG345 Chemical Engineering Laboratory I Spring 2021

- Conducted vapor-liquid equilibrium experiments for raw data collection
- Graded final project

Undergraduate Teaching Assistant

Physical Chemistry II — Fall 2018

- Held after-class Q&A sessions

Introductory Physics — Spring 2016

- Held after-class Q&A sessions

Publications

1. **Yu, K.**; Wang, C.; Zheng W.; Vlachos, D. G. Dynamic Electrification of Dry Reforming of Methane with *In situ* Catalyst Regeneration. Submitted.
2. **Yu, K.**; Srinivas, S.; Wang, C.; Chen, W.; Ma, L.; Ehrlich, S. N.; Marinkovic, N.; Kumar, P.; Stach, E. A.; Caratzoulas, S.; Zheng, W.; Vlachos, D. G. High-Temperature Pretreatment Effect on Co/SiO_2 Active Sites and Ethane Dehydrogenation. *ACS Catal.* **2022**, 11749–11760.
3. Wang, C.; **Yu, K.**; Sheludko, B.; Xie, T.; Kots, P. A.; Vance, B. C.; Kumar, P.; Stach, E. A.; Zheng, W.; Vlachos, D. G. A General Strategy and a Consolidated Mechanism for Low-Methane Hydrogenolysis of Polyethylene over Ruthenium. *Appl. Catal. B Environ.* **2022**, 319, 121899.
4. Fu, J.; Liu, S.; Zheng, W.; Huang, R.; Wang, C.; Lawal, A.; Alexopoulos, K.; Liu, S.; Wang, Y.; **Yu, K.**; Boscoboinik, J. A.; Liu, Y.; Liu, X.; Frenkel, A. I.; Abdelrahman, O. A.; Gorte, R. J.; Caratzoulas, S.; Vlachos, D. G. Modulating the Dynamics of Brønsted Acid Sites on $PtWO_x$ Inverse Catalyst. *Nat. Catal.* **2022**, 5 (2), 144–153.
5. Wang, C.; Xie, T.; Kots, P. A.; Vance, B. C.; **Yu, K.**; Kumar, P.; Fu, J.; Liu, S.; Tsilomelekis, G.; Stach, E. A.; Zheng, W.; Vlachos, D. G. Polyethylene Hydrogenolysis at Mild Conditions over Ruthenium on Tungstated Zirconia. *JACS Au* **2021**, 1 (9), 1422–1434.
6. Chen, W.; Malhotra, A.; **Yu, K.**; Zheng, W.; Plaza-Gonzalez, P. J.; Catala-Civera, J. M.; Santamaria, J.; Vlachos, D. G. Intensified Microwave-Assisted Heterogeneous Catalytic Reactors for Sustainable Chemical Manufacturing. *Chem. Eng. J.* **2021**, 130476.
7. Chen, W.; Cohen, M.; **Yu, K.**; Wang, H.-L.; Zheng, W.; Vlachos, D. G. Experimental Data-Driven Reaction Network Identification and Uncertainty Quantification of CO_2-Assisted Ethane Dehydrogenation over Ga_2O_3/Al_2O_3. *Chem. Eng. Sci.* **2021**, 237, 116534.
8. Suo, H.; Wang, W.; Jiang, S.; Li, Y.; **Yu, K.**; Huang, S.; Cui, S.; Shen, X.; Xue, J. Preparation of $ZrC@Al_2O_3@$Carbon Composite Aerogel with Excellent High Temperature Thermal Insulation Performance. *SN Appl. Sci.* **2019**, 1 (5), 461.

Presentations

1. **Yu, K.**; Srinivas, S.; Chen, W.; Wang, C.; Zheng, W.; Vlachos D. G.; Ethane Non-Oxidative Dehydrogenation over Co/SiO_2 —Effects of Pretreatment and Regeneration. *North American Catalysis Society Meeting*, **2022**. New York, NY. (Oral)
2. **Yu, K.**; Srinivas, S.; Chen, W.; Wang, C.; Zheng, W.; Vlachos D. G.; Synthesis, Optimization and Characterization of Co/SiO_2 for Ethane Dehydrogenation. *Catalysis Club of Philadelphia*, **2022**. (Oral)
3. **Yu, K.**; Srinivas, S.; Chen, W.; Wang, C.; Zheng, W.; Vlachos D. G.; Ethane Non-Oxidative Dehydrogenation over Co/SiO_2 — Pretreatment and Regeneration. *AICHE Annual Meeting*, **2021**. Boston, MA. (Poster)

Skills

Laboratory Instruments:
XRD, (NAP)XPS, XRF, FTIR, Raman, UV-Vis, TGA, GC, Mass spectrometer, Chemisorption station

Electron microscopy:
JEOL JEM-2010F TEM with *in situ* heating holder; JEOL NEORAM Cs-corrected STEM; Zeiss Auriga SEM with focused ion beam

Programing and Designing:
Python, MATLAB, LabView, Fusion 360, AutoCAD

MEHDI ZARE, PhD

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Proven chemical engineer, computational scientist, and researcher with 6+ years of research experience focusing on catalysis and interfacial phenomena using computational chemistry and machine learning. Experienced in simulation, modeling, and machine learning techniques; familiarized with catalyst synthesis, characterization methods, fabrication, testing, and inspection of fluid system assemblies. Currently, I am a postdoctoral researcher in Chemical Engineering Department at the University of Delaware, working towards developing next-gen catalysts for plastics recycling/upcycling using simulation and machine learning to guide the experimental synthesis route. I am looking for my next challenge – with employment opportunities in research or design in oil & gas, chemical, drug discovery, and science-based industries where I can continue to learn while contributing to a company's core mission.

RESEARCH EXPERIENCES

Postdoctoral Researcher, University of Delaware (Newark, DE, USA) (Aug.2021-present)

- Advisor: Dionisios G. Vlachos, PhD
- Developed a scheme to investigate conformational properties of polymers over catalyst surfaces employing statistical mechanics theory, enhanced sampling techniques such as Replica Exchange Molecular Dynamics (REMD) and Umbrella Sampling.
- Collaborated with experimentalists to design novel catalysts and processes for recycling/upcycling of plastic wastes.

Graduate Research Assistant, University of South Carolina (Columbia, SC, USA) (Aug.2016-Aug.2021)

- Developed a multiscale hybrid QM/MM model (eSMS) for catalysis at solid-liquid interfaces to enable long time molecular dynamics simulations with higher accuracy.
- Performed first-principles microkinetic modeling of hydrodeoxygenation of various biomolecules (e.g., methane, propane etc.) over transition metal catalysts in vapor and aqueous phases to identify the factors governing the reaction kinetics.
- Developed a graph neural network potential for the metal-water interaction and trained the model on in-house generated data.
- Developed an ML based model to quantify the solvent effect in heterogenous catalysis.

Graduate Student, University of Tehran (Tehran, Iran) (Sep.2011-Sep.2013)

- Conducted numerical simulation on liquid flow in the porous media using MATLAB software.
- Examined water transport in various GDL porous media using pore network modeling (PNM).
- Performed multiple course projects using Aspen Plus software.

Undergraduate Student, Shiraz University (Shiraz, Iran) (Sep.2007-Sep.2011)

- Designed and fabricated a ventilated steering wheel to improve driver's thermal comfort level.
- Optimized temperature and flow rate for enhanced thermal comfort using MATLAB.

RELATED INDUSTRY EXPERIENCES

Engineering Intern, Fars Combined Cycle Power Plant (Shiraz, Iran) (June-Sep 2011)

- Maintained and monitored power plant cycles and important units to detect anomaly during its normal operating hours.
- Collaborated with fellow interns (write a specific project) .
- Received hands on training on industrial equipment.

Design Engineer, PIDEC ***(Petrochemical Industries Design & Engineering Company)*** (Shiraz, Iran) (Feb-Aug 2016)

- Studied and analyzed different projects PFDs, BFDs, P&IDs, plot plans, etc.

CORE COMPETENCIES

Programming: Python, Fortran, MATLAB

Machine Learning: Scikit-learn, TensorFlow, Pytorch, RuNNer (a graph neural network code written in Fortran)
Quantum Chemistry: VASP, VASPsol, ASE, Dlpoly, LAMMPS, TURBOMOLE, COSMO, COSMO-RS
Experimental Chemistry: Familiar with catalyst synthesis and characterization
Chemical Engineering: Familiar with reactor design and operation

SELECTED PUBLICATIONS

M. Zare, P. A. Kots, S. Caratzoulas, D. G. Vlachos, "Conformations of polyolefins on platinum catalysts control product distribution in plastics recycling" (*under review*)

M. Zare, M. Saleheen, N. Singh, M. J. Uline, M. Faheem, A. Heyden, "Liquid-phase effects on adsorption processes in heterogeneous catalysis," *JACS Au* 2, 9: 2119–2134, **2022**

M. Zare, M. Saleheen, S. Kundu, A. Heyden, "Dependency of solvation effects on metal identity in surface reactions," *Communication Chemistry* 3: 187, **2020**

M. Zare, R.V. Solomon, W. Yang, A. Yonge, A. Heyden, "Theoretical Investigation of Solvent Effects on the Hydrodeoxygenation of Propionic Acid over a Ni(111) Catalyst Model," *The Journal of Physical Chemistry C*, 124: 16488–16500, **2020**

A.J. Chowdhury, W. Yang, K.E. Abdelfatah, **M. Zare**, A. Heyden, G.A. Terejanu, "A Multiple Filter Based Neural Network Approach to the Extrapolation of Adsorption Energies on Metal Surfaces for Catalysis Applications," *Journal of Chemical Theory and Computation* 16: 1105-1114, **2020**

K. Abdelfatah, W. Yang, R.V. Solomon, B. Rajbanshi, A. Chowdhury, **M. Zare**, S. Kundu, A. Yonge, A. Heyden, G. Terejanu, "Prediction of transition-state energies of hydrodeoxygenation reactions on transition-metal surfaces based on machine learning," *The Journal of Physical Chemistry C* 123: 29804-29810, **2019**

EDUCATION

PhD in Chemical Engineering, University of South Carolina (Columbia, SC, USA) (Aug.2021)

- GPA: 4.00/4.00
- Awarded Outstanding graduate student research award
- Dissertation title: "Solvent effect modeling in heterogenous catalysis"
- Advisor: Andreas Heyden, PhD

Master of Science in Chemical Engineering, University of Tehran (Tehran, Iran) (Sep.2013)

- GPA: 3.91/4.00 (ranked 3rd among graduate class of 2013)
- Dissertation title: "Analysis of water transport in GDL of PEMFC using PNM"
- Advisor: Ali Vatani, PhD and Gholamreza Karimi, PhD

Bachelor of Science in Chemical Engineering, Shiraz University (Shiraz, Iran) (Sep.2011)

- GPA: 3.22/4.00 (Top 10%)
- Thesis: "Experimental study of thermal comfort in the driver's hands with a ventilated steering wheel"
- Advisor: Gholamreza Karimi, PhD

REFERENCES

Dionisios G. Vlachos, PhD
University of Delaware
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Jiahua Zhou

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University of Delaware, Newark, Delaware 19716, United States
Mobile Phone: +1-302-608-4060 E-mail: jhzhou@udel.edu

Education

Ph.D. July 2019 – Present
Department of Chemical and Biomolecular Engineering, University of Delaware
Thesis topic: Fundamental investigation of the role of surface oxygen functional groups on carbon support as well as the inverse metal-metal oxide catalysts including materials synthesis and characterizations
Advisor: Prof. Dion Vlachos

M.Eng. September 2015 – May 2018
School of Chemical Engineering, Tianjin University
Thesis topic: Fabrication of PtSn-based catalysts for direct hydrogenation of acetic acid to ethanol
Advisor: Prof. Yujun Zhao

B.Eng. September 2011 – July 2015
School in Chemical Engineering & Technology, Wuhan University of Technology
Thesis topic: Mesoporous TiO_2/P3HT nanophotocatalyst for degradation of organic pollutants
Advisor: Prof. Yan Zhu

Teaching Experiences

September 2021 – December 2021 & March 2022 – June 2022
Teaching Assistant, Department of Chemical and Biomolecular Engineering, University of Delaware

Publications

1. **J. Zhou**[†], P. Yang[†], P. Kots, M. Cohen, Y. Chen, C. Quinn, M. Mello, J. Boscoboinik, W. Shaw, S. Caratzoulas, W. Zheng[*], D. G. Vlachos[*], "Tuning Oxygen-Containing Functional Groups and Reactivity of Carbon Surfaces", ***Submitted***.
2. **J. Zhou**, S. Deshpande, Y. Wang, J. Fu, W. Zheng[*], and D. G. Vlachos[*], "The Role of Metal Cores on the WO_x/M Inverse Catalysts", ***In preparation***.
3. Y. Wu, S. Sourav, A. Worrad, **J. Zhou**, S. Caratzoulas, G. Tsilomelekis, W. Zheng, D. G. Vlachos[*], "Dynamic Formation of Brønsted Acid Sites over WO_x-Pt Inverse Catalysts-A spectroscopic Investigation", ***In preparation.***
4. **J. Zhou**, W. Zheng[*], D. G. Vlachos[*], "Understanding the Role of Ni on $NiWO_x$ Inverse Catalysts", ***In preparation.***
5. Y. Hsiao, X. Zong, **J. Zhou**, W. Zheng, D. G. Vlachos[*], "Selective Hydrodeoxygenation of 5-hydroxymeylfurfural (HMF) over Carbon Supported Copper Catalysts Using Isopropyl Alcohol as a Hydrogen Donor", ***Applied Catalysis B: Environmental*** **2022**, 12, 121790.
6. Y. Wang, S. Lee, **J. Zhou**, J. Fu, A. Foucher, E. Stach, L. Ma, N. Marinkovic, S. Ehrlich, W. Zheng[*], D. G. Vlachos [*], "Higher Loading of Pt Single Atoms and Clusters over Reducible Metal Oxides: Application to C-O Bond Activation", ***Catalysis Science & Technology*** **2022**, 12, 2920-2928.
7. D. Pan[†], **J. Zhou**[†], B. Peng[*], S. Wang, Y. Zhao[*], X. Ma, "The Cooperation Effect of Ni and Pt in the Hydrogenation of Acetic Acid", ***Frontiers of Chemical Science and Engineering*** **2022**, 16, 397-407.

8. **J. Zhou**, Y. Zhao*, J. Zhang, Y. Wang, O. Y. Gutierrez, S. Wang, Z. Li, P. Jin*, S. Wang, X. Ma, J. A. Lercher, "A Nitrogen-doped PtSn Nanocatalyst Supported on Hollow Silica Spheres for Acetic Acid Hydrogenation", ***Chemical Communications*** **2018**, 54, 8818-8821. **(Back Cover Story)**
9. Y. Zhao*, X. Wu, **J. Zhou**, Y. Wang, S. Wang, X. Ma, "MOF-derived Cu@C Catalyst for the Liquid-phase Hydrogenation of Esters", ***Chemistry Letters*** **2018**, 47, 883-886.
10. Y. Zhao*, B. Shan, Y.Wang, **J. Zhou**, S. Wang, X. Ma, "An Effective CuZn-SiO_2 Bimetallic Catalyst Prepared by Hydrolysis Precipitation Method for the Hydrogenation of Methyl Acetate to Ethanol", ***Industrial & Engineering Chemistry Research*** **2018**, 57, 4526-4534. (Cover Story)

International Presentations

1. **J. Zhou**, P. Yang, W. Zheng, and D. G. Vlachos*, "The Role of Oxygen-Containing Functional Groups of Carbon Surfaces", 2022 The 27th North American Catalysis Society Meeting, Poster Presentation, May. 22-27, 2022.
2. **J. Zhou**, W. Zheng*, and D. G. Vlachos*, "The Role of Oxygen-Containing Functional Groups of Carbon Surfaces", 2021 AIChE Annual Meeting, Virtual Poster Presentation, Nov. 15-19, 2021.

Awards and Honors

1. **Outstanding Master`s Thesis Winner of Tianjin University, 2018**
2. Tianjin University Second-class scholarship, 2016 & 2017
3. Tianjin University-level All-round Excellent Student, 2016
4. Tianjin University First-class scholarship, 2015
5. **Outstanding Graduate of Wuhan University of Technology, 2015**
6. **Outstanding Bachelor`s Thesis Winner of Hubei Province, 2015**
7. PPG scholarship, Wuhan University of Technology, 2013~2014
8. First-class scholarship, Wuhan University of Technology, 2013~2014 & 2012~2013
9. Wuhan University of Technology-level All-round Excellent Student, 2013~2014, 2012~2013
10. Third-class scholarship, Wuhan University of Technology, 2011~2012
11. Outstanding Student Leader, Wuhan University of Technology, 2011~2012

Technical Skills

1. Material Design and Synthesis
   - M-MO_x inverse Catalysts (M = Pt, Ru, Rh, Pd, Au, Co, Ni)
   - Oxygen functionalized Carbon materials
2. Characterization Techniques
   - XPS, AP-XPS, TEM, Raman spectroscopy, TPR & TPD
   - Physisorption, Chemisorption, TEM, TGA, XRD, SEM
3. Reactor Design and Operation
   - Fixed-bed flow reactor for continuous dehydration reactions

DEPARTMENT OF CHEMICAL & BIOMOLECULAR ENGINEERING