Mohammed Al Otmi

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EDUCATION

University of Florida Gainesville, FL

Ph.D. & M.S. in Chemical Engineering, GPA: 3.97 Aug 2020 – May 2025

- Thesis: Understanding Transport Mechanisms in Polymer Membranes Through Molecular Simulations
- Workshops: ML for Molecular Science (i-CoMSE), Lab-scale Reactor Design (Dow), Data-driven Material Innovation (Schrodinger), Supervised Machine Learning (DeepLearningAI)

Mississippi State University Starkville, MS

B.S. in Chemical Engineering, GPA: 3.73 Aug 2016 – May 2019

- Minor in Political Science, AIChE Safety & Chemical Engineering (SAChE) Certificate, Dean's Scholar

PROFESSIONAL EXPERIENCE

Energy Frontier Research Center (EFRC) Remote

Computation & Informatics Researcher Dec 2022 – Present

- Led DOE-funded AEMFC projects, managing timelines and delivering 4 conference presentations.
- Collaborated within a multidisciplinary team to design fluorine-rich poly(arylene amine) membranes with up to 10x energy/cost savings for hydrocarbon separations.
- Used MD + ML to screen 11M copolymers, revealing transport physics of top candidates.
- Devised a model capturing ion correlation/proton hopping in AEM, improving simulation-experiment agreement.

University of Florida Gainesville, FL

Graduate Research Assistant Aug 2020 – May 2025

- Built a high-throughput MD/MC framework for analyzing free volume in polymer membranes.
- Illustrated the correlation between segmental dynamics to free volume element stability and penetrant diffusion.
- Developed a QSPR ML model predicting density and T_g from 13k+ homopolymers.

Delta Protein International Sunflower, MS

Product Quality Engineering Intern May 2020 – Aug 2020

- Used HPLC to characterize collagen hydrolysates, ensuring controlled enzymatic breakdown into low molecular weight peptides (5 kDa) $< 5\,\mathrm{kDa}$, for enhanced solubility and bioavailability.
- Conducted daily quality tests: pH, viscosity, conductivity, color, standard plate count (SPC), etc.
- Created GMP-compliant SOP; implemented AVEVA Historian for real-time quality tracking.

Mississippi State University Starkville, MS

Undergraduate Researcher Aug 2018 – May 2019

- Synthesized dithiocarbamate-modified polystyrene resin; enhanced structural stability by 40% through crosslinking and verified structure via FTIR.
- Used Atomic Absorption Spectroscopy to measure heavy metal removal capacity; achieved up to 20% efficiency.

TECHNICAL SKILLS

- **Programming & Scripting:** Python, Bash, High-Performance Computing (HPC)
- **Machine Learning & Modeling:** Scikit-learn, Bayesian Optimization, QSPR Models
- **Computational Chemistry:** Molecular Dynamics (LAMMPS, GROMACS), Monte Carlo, DFT (Gaussian)
- **Experimental & Analytical Tools:** HPLC, AAS, FT-IR, DOE, Post-polymerization Functionalization
- **Process Engineering:** Scale-up, equipment sizing, PFDs, P&IDs, troubleshooting, technoeconomic analysis
- **Software & Platforms:** AVEVA Historian, Git, LaTeX, Microsoft Office Suite, CHEMCAD
- **Languages:** English (Professional Proficiency), Arabic (Professional Proficiency)

LEADERSHIP & MENTORSHIP

- Led AEM projects at EFRC; coordinated goals, teams, and reporting.
- Trained 6+ students; created lab manuals and software tutorials.
- Teaching assistant & guest lecturer for Separations and Mass Transfer Operations class; Spring 2023.
- Treasurer and sport chair, Graduate Association of Chemical Engineers (GRACE); peer mentor for incoming students.
- Helped establish the Yemeni Student Association at MSU; hosted a cultural showcase with 1,500+ attendees.

SELECTED AWARDS

- 2024 AICHE Excellence Award in Graduate Polymer Research, UF Research Excellence Fellowship
- 2023 Elias Klein Founder's Award from North American Membrane Society
- 2018 Winner of MSU Undergraduate Research Stipend
- 2016 Phi Theta Kappa Scholarship, Maron & White Scholarship
- 2013 The Top-Ten Student scholarship for undergraduate studies from the Yemeni government

PUBLICATIONS

- Al Otmi, M., Colina, C., Lively, R., Sampath, J. "Free Volume Elements in Polymer Membranes: Theory, Characterization, Functional Significance, and Design Strategy." ***Book Chapter in Computational Methods for the Multiscale Modelling of Soft Matter***, **Elsevier Inc**, In Press.
- Schertzer, W., Shukla, S., Rafiq, R., Al Otmi, M., . . . , Ramprasad, R. "AI-Driven Design of Fluorine-Free Polymers for Sustainable and High-Performance Anion Exchange Membranes." ***Journal of Materials Informatics***, 2025.
- Yi, R., Hui, M., Kim, J., Al Otmi, M., . . . , Sampath, J., Realff, M., Lively, R., Guo, S. "Fluorine-Rich Poly(Arylene Amine) Membranes for the Separation of Liquid Aliphatic Compounds." ***Science***, 2025.
- Al Otmi, M., Lin, P., Schertzer, W., Colina, C., Ramprasad, R., Sampath, J. "Investigating Correlations in Hydroxide Ion Transport in Anion Exchange Membranes from Atomistic MD Simulations." ***ACS Applied Polymer Materials***, 2024.
- Al Otmi, M.*, Wernisch, B.*, Sampath, J. "Evolution of Free Volume Elements in Amorphous Polymers Undergoing Uniaxial Deformation" ***Molecular Systems Design & Engineering***, 2024. (*equal contribution)
- Al Otmi, M., Willmore, F., Sampath, J. "Structure, Dynamics, and Hydrogen Transport in Amorphous Polymers: An Analysis of the Interplay Between Free Volume Element Distribution and Local Segmental Dynamics from Molecular Dynamics Simulations." ***Macromolecules***, 2023.

CONFERENCES & PRESENTATIONS

- **American Institute of Chemical Engineers (AIChE) Annual Meeting**
  - *Probing Polymer Relaxation Dynamics Using MD Simulations*. Oral Presentation, 2024, San Diego, CA.
  - *Exploring the Contributions of Vehicular and Grotthuss Diffusion Mechanisms in Anion Exchange Membranes*. Poster, 2024, San Diego, CA.
  - *Investigating Ion Transport, Mechanical Properties, and Stability of Tetraalkylammonium-Functionalized Polyethylene*. Oral Presentation, 2023, Orlando, FL.
  - *Effect of Chain Dynamics on the Free Volume Elements of Glassy Polymers from Atomistic Molecular Dynamics Simulations*. Oral Presentation, 2022, Phoenix, AZ.
- **Foundations of Molecular Modeling and Simulation (FOMMS)**
  - *Navigating Polymer Membrane Design: Balancing Durability and Performance*. Poster, 2024, Snowbird, UT.
- **North American Membrane Society (NAMS)**
  - *Modeling Permeation in Polymer Membranes Using Non-Equilibrium Molecular Dynamics Simulations*. Oral Presentation, 2023, Tuscaloosa, AL.
- **National Organization for the Professional Advancement of Black Chemists and Chemical Engineers (NOBCChE)**
  - *Unraveling Membrane Mysteries: Molecular Insights for Polymer Design in Gas Separation and Ion Exchange Applications*. Oral Presentation, 2024, Orlando, FL.
- **UF GRACE Symposium**
  - *Atomistic Modelling of Hydrogen Diffusion in Polystyrene, Polymethylpentene, and HAB-6FDA Thermally Rearranged Polymers*. Oral Presentation, 2022, Gainesville, FL.
- **33rd IUPAP Conference on Computational Physics (CCP)**
  - *The Dynamic Nature of Free Volume Element and its Effect on the Performance of Glassy Polymers Using Atomistic Molecular Dynamics Simulations*. Oral Presentation, 2022, Austin, TX.
- **Mississippi Water Resource Conference (MWRC)**
  - *Experimental Study of the Performance of the N,N'-di(carboxymethyl) dithicarbamate Chelating Resin in Removing Heavy Metals from Oilfield Wastewater*. Poster Presentation, 2019, Jackson, MS.

REFERENCES

- **Prof. Janani Sampath**, Assistant Professor
  Chemical Engineering Department
  University of Florida, Gainesville, FL, USA
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  Profile: Personal Page
- **Dr. Maryam Mirbolghasemi**, Lecturer
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- **Dr. Kirk Ziegler**, Professor
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  Profile: Personal Page
- **Dr. Jason Gorski**, General Manager
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