Jay Shah

SOFT MATTER | SIMULATIONS | MACHINE LEARNING

302-9326175 | jayshah@udel.edu | https://github.com/Jay-Shah1 | https://www.linkedin.com/in/jayshah-iit/

Education

University of Delaware *Delaware, US*

PHD IN CHEMICAL ENGINEERING, GPA: 3.9/4 *2022 - Present*

Indian Institute of Technology Gandhinagar *Gandhinagar, India*

B.TECH. IN CHEMICAL ENGINEERING, CPI: 8.47/10 *2018 - 2022*

Research Work

Understand polysulfmaide and polysulfmate morphology using molecular simulation

ADVISOR: PROF. ARTHI JAYARAMAN, UNIVERSITY OF DELAWARE *Jan. 2023 - Present*

- Utilized coarse-grained and atomistic molecular dynamics simulations to link polysulfamide chain design to the assembled structure's features
- Extended CG model to atomistically informed models using GROMACS, elucidating assembly outcomes and hydrogen bonding arrangements
- Investigated phase separation and blending morphology, revealing insights into miscibility and domain formation based on backbone chemistry and sulfamide group placement
- Developing machine learning approaches for analyzing data from experimental polarized optical microscopy images, differential scanning calorimetry, and wide angle X-ray scattering from polymeric materials

Publications and Conference

J. Shah, A. Jayaraman, **Coarse-grained molecular dynamics simulations of mixtures of polysulfamides**, *RSC Applied Polymers* [#]

J Shah, Z Wu, A Jayaraman , **Understanding self-assembly of polysulfamides from molecular dynamics simulations using atomistically-informed coarse grained models**, *AIChE Annual Meeting 2024*

J. Shah*, A. Paruchuri*, L. Nagidi, S. Lu, A. Jayaraman, **Linking polysulfamide design to morphology using molecular simulation and machine learning**, *APS March Meeting 2024*

J Shah*, Z Wu*, A Jayaraman , **Computational Studies to Understand the Effect of Polysulfamide Designs on Structure and Properties**, *MRS Fall meeting 2023*

C Ghoroi, **J Shah***, D Thakar* and S Baheti*, **Process design and economics of production of p-Aminophenol**, *arXiv, Cornell University Library*, DOI: arXiv:2110.15750, Oct. 2021.

* indicates equal contribution, # - manuscript is under review

Teaching Experience

Fall 2024	**TA - Molecular Modeling and Simulation of Soft Materials**, Prof. Arthi Jayaraman, University of Delaware	*United States*
Summer 2024	**Teaching Certificate, NRT Midas**, University of Delaware	*United States*
Spring 2022	**TA - Process Control**, Prof. Pratyush Dayal, IIT Gandhinagar	*India*
Fall 2022	**Teaching Certificate**, IIT Gandhinagar	*India*
Spring 2021	**TA - Fluid Mechanics Lab**, Prof. Prachi Thareja , IIT Gandhinagar	*India*

Experiences

Molecular dynamics simulation study of shock wave deformation in polyethylene

GUIDE: PROF. RAGHAVAN RANGANATHAN, IIT GANDHINAGAR *Aug. 2021 - March 2022*

- Simulated the shock wave propagation in polyethene using rigid piston method to understand the thermodynamical change in the materials
- Studied the damping properties of polymer nanocomposites to observe the enhancement in the property of the bulk due to nanoparticles fillers

Network anomaly detection in Water distribution network, University of Miami

MENTOR: PROF. RAMIN MOGHADDASS, UNIVERSITY OF MIAMI *June 2021 - Aug. 2021*

- Built a simulation framework for network anomaly detection in large-scale water networks using synthetic data to validate and test the model.
- Developed a hierarchical method utilizing three deep neural networks to compress information from network topology, network status, and sensor data for anomaly detection.
- ***Submitted conference paper IISE Annual Conference and Expo, Seattle 2022***

Modelling of Cavity Growth in underground coal gasification, IIT Madras

MENTOR: PROF. PREETI AGHALAYAM, IIT MADRAS   *May 2021 - July 2021*

- Built a MATLAB model of the Underground Coal Gasification cavity to predict the composition of the output gas by solving radial and time-variant ODEs
- The model is validated by comparing it with the literature results of laboratory-scale experiments. The model predicts the radial and time variation of the product gases inside the cavity
- *Accepted Abstract for Presentation at ICCCT conference, 2022*

Research and Development Intern, NEC LABS

MANAGER: MR. SACHIN MISHRA   *May 2020 - July 2020*

- Developed a web application to track family members' health records, ensuring easy access and management of medical histories.
- Engineered a machine learning model to detect diseases based on symptoms entered by users, using synthetic disease data provided by the company. Enhanced the user interface for better usability and experience and conducted comprehensive market research to guide product development and refinement.

Inventor, Invention Factory-INVENT@IITGN,2019 by Cooper Union USA and IIT-GN

MENTOR: PROF. ALAN WOLF AND PROF. ERIC LIMA, COOPER UNION, NEW YORK   *May 2019 - June 2019*

- Designed a self-adjusting, automatic sun Visor and solar shade system for vehicles that determines the blocking needs of an individual driver in bright sunlight that prevent accidents
- Learned to use Arduino and integrating sensors to create custom electronic solutions. Learned 3D printing techniques, enabling rapid proto-typing.
- *File Patent Application for Indian (No.201921027106) and US Provisional Patent (EFS Id-37376706, Application Number - 62911388, Confirmation Number -1074)*

Projects

Understanding data handling in Molecular simulation   *University of Delaware*

MENTOR: PROF. SUNITA CHANDRASEKARAN   *Sept. 2024 - Dec. 2024*

- Analyzed simulations by tracking key metrics such as cache performance, latency, bandwidth, and leveraging Roofline Analysis to pinpoint memory or compute bottlenecks.
- Gained hands-on experience with benchmark suites, performance profilers, and executing code on various NVIDIA and AMD HPC systems.

Generative modelling of height maps for surface property engineering and design   *University of Delaware*

MENTOR: DR. ALEX BOURQUE, DR. MATTHEW MILLS, DR. STEVEN KONG   *Jan. 2024 - April 2024*

- Investigated the relationship between surface topography and material properties (adhesion, clarity, cleanability) using height maps recorded o by experimental methods, including confocal microscopy and atomic force microscopy
- Developed generative models and a machine learning workflow to create and optimize computer-generated height maps tailored to specific property requirements
- Implemented a diffusion model to generate height maps with desired properties, allowing for the integration of additional property sets into the workflow

Process Analysis and Simulation of Production of P-Aminophenol   *IIT Gandhinagar*

MENTOR: PROF. CHINMAY GHOROI   *Jan. 2021 - April 2021*

- Simulated the production of para aminophenol, using nitrobenzene and hydrogen as the raw material
- Developed the entire process for the reaction and separation method using ASPEN simulation
- Performed an economic analysis of the industrial plant for the process and calculate the payback period, return of investment

Computational Fluid Dynamics   *IIT Gandhinagar*

GUIDE: PROF. DILIP SUNDARAM   *Aug. 2020 - Dec. 2020*

- Understand and apply numerical analysis on 1-D steady and unsteady convection-diffusion equations using finite difference methods
- Developed the code for the solution of the Lid-Cavity flow problem. We used a 2-D Navier Stokes equation, using a finite volume method on a collocated grid with uniform cells for a laminar flow

Achievements

2024	**Outstanding contributions to NRT MIDAS** , University of Delaware	*United States*
2024	**Best technical project** , ATOM Hackathon	*United States*
2023	**Morton and Donna Collins Chemical Engineering Fellowship**, Chemical engineering grad student award	*United States*
2021	**Dean's List - Semester 5**, IIT Gandhinagar	*India*
2020	**Outstanding Project Certificate - Engineer's Conclave, Inter IIT Tech Meet 8.0**, IIT Roorkee	*India*

Technical Knowledge

Programming Language: Python *Libraries:* OpenCV, Numpy, Pandas, Tensorflow, Bash

Tools: LAMMPS, GROMACS, Aspen, MATLAB, AutoCAD, LaTeX