

Sree Harsha Bhimineni

Email : sreeharshabhimineni@gmail.com; Mobile : (310) 696-6038; LinkedIn : sreeharshabhimineni

EDUCATION

University of California, Los Angeles

Ph.D. Chemical Engineering, Sautet Research Group

M.S. Chemical Engineering, Sautet Research Group

CGPA: **3.914/4**

Los Angeles, USA

2022 - 2027

2022 - 2024

National Institute of Technology, Warangal

B.Tech. Chemical Engineering

CGPA: **9.46/10** (Rank 1 among more than 1000 students)

Warangal, India

2018 - 2022

PUBLICATIONS

- Bhimineni, S. H.; Ko, S. T.; Cornwell, C.; Xia, Y.; Tolbert, S. H.; Luo, J.; Sautet, P. First Principles Study of Aluminum Doped Polycrystalline Silicon as a Potential Anode Candidate in Li-ion Batteries. *Advanced Energy Materials*, 10.1002/aenm.202400924 (**2024**)
- Bhimineni, S. H.; Zhou, T.; Mahmoodpour, S.; Singh, M.; Li, W.; Bag, S.; Sass, I.; Müller-Plathe, F. Machine-Learning-Assisted Investigation of the Diffusion of Hydrogen in Brine by Performing Molecular Dynamics Simulation. *Industrial and Engineering Chemistry Research*, 10.1021/acs.iecr.3c01957 (**2023**)

PROJECTS

Materials Screening for Pseudocapacitors

Prof. Philippe Sautet's lab, CBE Department, UCLA

Los Angeles, USA

March 2024 - Present

- Investigating a wide set of materials for pseudo-capacitive behavior. DFT and machine learning are used to understand the effect of different properties of the materials on their performance.

Silicon as a Potential Anode Candidate in Li-ion Batteries

Prof. Philippe Sautet's lab, CBE Department, UCLA

Los Angeles, USA

January 2023 - Present

- Developed a GitHub repository named **scalar_codes** that automates VASP and VASP-related calculations.
- Worked on improving the electrochemical performance of the silicon electrode by modifying it with aluminum which segregates in its grain boundaries and surfaces using DFT.
- Developed a grain boundary sliding model and performed simulations using VASP executed on high-performance computing clusters to understand the effect of aluminum on sliding. A **significant reduction (~ 90 %) in the sliding barrier** correlates to reduced internal stress development and reduced probability of failure.
- Constructed a hybrid solvation surface model using VASPsol to assess aluminum's effect on SEI formation, revealing its thermodynamically favorable SEI formation and adsorption, indicating reduced unstable growth.

Production of Epoxy Resins

Prof. Shirish H. Sonawane, ChE Department, NIT Warangal

Warangal, India

Jan 2022 - May 2022

- Devised a flow sheet for a continuous process for the synthesis of DGEBA; investigated a kinetic model for the polymer reaction using literature, modeled the system using mass and energy balances using MATLAB.
- Studied the effect of various parameters on the epoxy and phenolic content of the formed polymer.

Modelling of Forest Fire

Jha research group in the ChE Department, IIT Roorkee

Roorkee, India

Dec 2021 - Feb 2022

- Simulated forest fires using a model developed based on the Monte Carlo technique and implemented using Python.
- Obtained fire propagation data; fitted the data with a Weibull curve and studied the significance of model parameters.

Diffusivity Studies of Hydrogen in Brine

Müller-Plathe group in the Theoretical Physical Chemistry Department, TU Darmstadt

Darmstadt, Germany

May 2021 - Aug 2021

- Investigated the diffusivity of hydrogen in brine using a computational framework combining molecular dynamics simulations and machine learning for storage in aquifers as an energy storage application.
- Generated data using LAMMPS executed on high-performance computing clusters and integrated obtained data with machine learning using Python, achieving a fitting accuracy with an **R² score of 0.996**.

TECHNICAL SKILLS

Programming: Python (PyTorch, Scikit-Learn, Scipy, Numpy, Pandas, Matplotlib, OS, Subprocess, Argparse), MATLAB, C++, Bash, Git, High-Performance Computing, LaTeX

Simulation and Design: VASP, ASE, LAMMPS, Aspen Plus, DWSIM, AutoCAD

ACHIEVEMENTS

Institute gold medal; Best student award by Indian Institute of Chemical Engineers; Merit Scholarship for four consecutive years; Winner of elocution competition