Nikhil Kumar Thota

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Education

Ph.D Chemical and Biomolecular Engineering Expected Dec 2025
Johns Hopkins University, Baltimore, MD, USA

M.S.E Chemical and Biomolecular Engineering Dec 2021
Johns Hopkins University, Baltimore, MD, USA

B.Tech Chemical Engineering May 2019
Manipal Institute of Technology, Manipal, Karnataka, India

Skills

Regression and Classification Models : Neural Networks, Autoencoders, XGBoost, Gaussian Processes
Optimization Methods : Reinforcement Learning, Bayesian Optimization
Coding Languages (Packages) : Python (PyTorch, TensorFlow, NumPy), Bash, MATLAB (SimBiology, Parallel Computing), LaTeX, Markdown
Simulation Software : NAMD, **Visualization Software :** VMD, PyMOL, OVITO

Research and Professional Experience

Ph.D. Candidate Jan 2022 – Present
Rigoberto Hernandez Lab, Johns Hopkins University, Baltimore, MD, USA

- Developed and implemented a novel autoencoder (AE) model and training algorithm to construct material embeddings from high dimensional datasets which demonstrated a 20% improvement in power conversion efficiency prediction of metal halide perovskite (MHP) solar cells over a conventional AE while having an order of magnitude smaller error bounds.
- Developed and implemented a multi-agent reinforcement learning model to extract sparse feature sets from high dimensional datasets to reduce model overfitting. Model achieved most sparse feature set compared to XGBoost and LASSO while having lowest prediction error for DFT computed MHP bandgaps.

Ph.D. Intern Jul 2024 – Sep 2024
Pacific Northwest National Lab, Richland, WA, USA

- Developed a bayesian machine learning model to predict binding free energies of polypeptoid sequences to calcite surfaces to infer whether the polypeptoid sequence accelerates or inhibits calcite growth.
- Mentored a high school student on fundamentals of calculus and introductory python programming.

M.S.E Student Jul 2019 – Aug 2020
Rigoberto Hernandez Lab, Johns Hopkins University, Baltimore, MD, USA

- Analysed and contrasted protein unfolding energetics of a wildtype Actophorin to a mutant Actophorin using adaptive steered molecular dynamics.
- Identified mutated residues responsible for increased chemical and thermal stability of Actophorin.

Process and Safety Engineer Aug 2020 – Dec 2021
ExxonMobil Services and Technology Private Limited, Bengaluru, Karnataka, India

- Executed consequence analysis calculations to determine dispersion radius and concentration of flammable materials from vessels with various leak sizes. Scribed risk assessment meetings.
- Evaluated and contrasted different technologies for treating crude oil emulsions for XTO Energy. Conceptualized and designed a heater treater unit for their operations.

Undergraduate Intern Jan 2019 – Dec 2019
Toley Lab, Indian Institute of Science, Bengaluru, Karnataka, India

- Identified reaction products and pathways involved in loop mediated and isothermal amplification (LAMP) of

DNA used in PCR free diagnosis kits of tuberculosis and COVID-19.

- Developed an algorithm to simulate the devised stoichiometric model and validated model outputs using experimental gel electrophoresis images and fluorescence readouts.

Teaching Experience

Instructor for EN.540.635 Software Carpentry Sep 2024 – Dec 2024
Johns Hopkins University, Baltimore, MD, USA

- Taught introductory python programming and applications to a class of 30 students.
- Held office hours to resolve student queries and guided students during their midterm and final projects.
- Managed a team of one graduate TA and grader to handle grading of weekly homeworks and projects.

Instructor for Python Summer School Jul 2023 – Aug 2023
Virtual (https://scotch.wangyq.net)

- Volunteered to teach basics of machine learning using PyTorch in summer school led by Dr. Pratyush Tiwary.

Graduate Teaching Assistant for EN.540.409.01 for Process Dynamics and Control Jul 2023 – Aug 2023
Johns Hopkins University, Baltimore, MD, USA

Publications

1. Priyadarshini, M. S.; **Thota, N. K.**; Hernandez, R. ReLMM: Reinforcement Learning Optimizes Feature Selection in Modeling Materials. *J. Chem. Inf. Model.* **2025**, 65 (1), 153–161. DOI: 10.1021/acs.jcim.4c01934
2. **Thota, N. K.**; Priyadarshini, M. S.; Hernandez, R. NestedAE: Interpretable Nested Autoencoders for Multi-Scale Materials Characterization. *Mater. Horiz.* **2024**, 11 (3), 700–707. DOI: 10.1039/D3MH01484C.
3. **Thota, N. K.**; Quirk, S.; Zhuang, Y.; Stover, E. R.; Lieberman, R. L.; Hernandez, R. Correlation between Chemical Denaturation and the Unfolding Energetics of Acanthamoeba Actophorin. *Biophysical Journal* **2022**, S0006349522038590. DOI: 10.1016/j.bpj.2022.11.2941
4. Zhuang, Y.; **Thota, N. K.**; Quirk, S.; Hernandez, R. Implementation of Telescoping Boxes in Adaptive Steered Molecular Dynamics. *J. Chem. Theory Comput.* **2022**, 18 (8), 4649–4659. DOI: 10.1021/acs.jctc.2c00498
5. Kaur, N.; **Thota, N. K.**; Toley, B. J. A Stoichiometric and Pseudo Kinetic Model of Loop Mediated Isothermal Amplification. *Comput. Struct. Biotechnol. J.* **2020**, 18, 2336–2346. DOI: 10.1016/j.csbj.2020.08.020

Conference Presentations

1. **Thota, N. K. (Presenter)**, Priyadarshini, M. S., Hernandez, R *Multiscale Modeling of Materials Using Nested Autoencoders*. Presented at the AI-X Foundry Symposium, Johns Hopkins University, Baltimore, MD, Sep 27, 2023 Abstract
2. **Thota, N. K. (Presenter)**, Quirk, S.; Zhuang, Y.; Hernandez, R. *Mutational Assay of an Actophorin Protein Using Adaptive Steered Molecular Dynamics*, Presented at American Chemical Society Conference, Chicago, IL, Aug 22, 2022 Abstract

Select Awards and Certificates

1. Graduate TA award for EN.540.635 Software Carpentry — Apr 2025
2. Department travel award for Fall 2022 ACS Conf. — Jun 2022
3. Finalist in Empower Your Pitch competition (3 minute research communication) — Apr 2022
4. Department scholarship for second year of M.S.E program — Sep 2021

Academic Service and Leadership

Executive Board Member in Graduate Student Liason Committee (GSLC) Sep 2022 – Sep 2023
Johns Hopkins University, Baltimore, MD, USA

- Facilitated two way communication between the graduate student in the department and the university wide Graduate Research Organization (GRO).
- Organized student led seminars and 30+ social activities for graduate students in the department.