Nikhil Kumar Thota

Baltimore, MD | nthota2@jhu.edu | +1 443-889-4827 | Website | Linkedin | Github

Education

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

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

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

Research Experience

Ph.D. Candidate　　　　　　　　　　　　　Jan 2022 – Present
Advisors: Dr. Rigoberto Hernandez (Johns Hopkins), Dr. Paulette Clancy (Johns Hopkins)

- Developed novel autoencoder (AE) model (NestedAE) to construct material embeddings from high dimensional, multimodal datasets for material discovery.
- Applied model to predict power conversion efficiencies (PCE) of metal halide perovskites (MHP) by combining datasets containing bandgaps computed using density functional theory (DFT) and JV characterized solar cells.
- Demonstrated 20% improvement in PCE prediction of MHP solar cells with smaller error bounds over conventional supervised AE. Identified ionic species that maximize PCE using Bayesian Optimization.
- Presented "Discovery of New Solar Cell Material using Deep Learning" to university wide audience in under 3 minutes in 2022 Empower Your Pitch (EYP) competition.
- Co-developed a multi-agent reinforcement learning model to extract sparse feature sets from high dimensional datasets for improved interpretability and predictive models.
- Demonstrated model achieves feature set size 40 percent smaller than XGBoost while having lower or comparable prediction errors for DFT computed MHP bandgaps.

M.S.E Student　　　　　　　　　　　　　Sep 2020 – Dec 2021
Advisor: Dr. Rigoberto Hernandez (Johns Hopkins)

- Co-developed a novel simulation method to reduce run time of steered molecular dynamics (SMD) simulations to compute potential of mean force of unfolding for large proteins by introducing variable size solvent boxes.
- Demonstrated method to analyse and contrast protein unfolding energetics of a wildtype Acanthamoeba Actophorin protein to mutated variant. Identified mutated residues and their interactions responsible for increased chemical and thermal stability of protein.
- Wrote Bash and Python scripts to simulate and analyse simulations on Johns Hopkins HPC cluster.

Undergraduate Intern　　　　　　　　　　　　　Jan 2019 – Dec 2019
Advisor : Dr. Bhushan Toley (Indian Institute of Science, Bengaluru, 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 Software Carpentry　　　　　　　　　　　　　Sep 2024 – Dec 2024
Johns Hopkins University, Baltimore, MD

- Taught introductory python programming and applications to 30 graduate students, resolved student queries and guided students during their midterm and final projects.
- Managed course website through Github and supervised a team of a graduate TA and grader to handle grading of weekly homeworks and projects and hold office hours.

Instructor for Python Summer School — Jul 2023 – Aug 2023

Virtual (https://scotch.wangyq.net)

- Volunteered to teach an hour long session using google collab notebooks to 20 students with varied backgrounds on tensor operations and backpropagation using PyTorch in summer school led by Dr. Pratyush Tiwary.

Teaching Assistant for Process Dynamics and Control — Sep 2022 – Dec 2022

Johns Hopkins University, Baltimore, MD

- Graded undergraduate weekly assignments and tutored 17 undergraduates during weekly recitation sessions.
- Presented to class of 70 plus undergraduates on applications of machine learning in process control.

Select Publications

1. Baird, S.; ... **Thota, N. K.**; ... Zou, Y. Bayesian Optimization Hackathon for Chemistry and Materials. *ChemRxiv*, June 23, 2025. DOI: 10.26434/chemrxiv-2023-tkcd9

2. 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

3. **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.

4. **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

5. 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

6. 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

Select 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. Department Graduate TA award for Software Carpentry — Apr 2025
2. Finalist in 2022 EYP competition. — Apr 2022

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 graduate students 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.

Skills

Regression and Classification Models : 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