**Nikhil Kumar Thota**

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## Education

**Ph.D. in Chemical and Biomolecular Engineering** — Jan 2022 – Present
*Johns Hopkins University, Baltimore* — Maryland, USA

**M.S.E in Chemical and Biomolecular Engineering**, GPA: 3.85/4.00 — Sep 2020 – Dec 2021
*Johns Hopkins University, Baltimore* — Maryland, USA

**B.Tech. in Chemical Engineering**, GPA: 8.69/10.00 — Jul 2015 – May 2019
*Manipal Institute of Technology, Manipal* — Karnataka, India

## Employment History

**Ph.D. Student** in Chemical and Biomolecular Engineering — Jan 2022 – Present
*Hernandez Lab, Johns Hopkins University, Baltimore* — Maryland, USA

- Ongoing thesis : "Data Driven Algorithms for Multiscale Design and Synthesis"
- Developed learning algorithms for multiscale design of materials. The models have demonstrated capabilities to predict and design hybrid Metal Halide Perovskites with improved power conversion efficiencies.

**Ph.D. Intern - Material Science** — Jul 2024 – Sep 2024
*Pacific Northwest National Lab, Richland* — Washington, USA

- Developed machine learning models to correlate the kinetics of calcite crystal nucleation and growth to either step-pinning, incorporation or kink blocking mechanism.

**M.S.E Student** in Chemical and Biomolecular Engineering — Sep 2020 – Dec 2021
*Hernandez Lab, Johns Hopkins University, Baltimore* — Maryland, USA

- Thesis: "Correlation Between Chemical Denaturation and the Unfolding Energetics of *Acanthamoeba Actophorin*"
- Utilized an in house developed code called Adaptive Steered Molecular Dynamics (ASMD) to investigate and contrast the protein unfolding energetics of a wildtype and mutant protein called *Acanthamoeba Actophorin*.

**Process and Safety Engineer** — Jul 2019 – Aug 2020
*ExxonMobil Services and Technology Private Limited, Bengaluru* — Karnataka, India

- Worked on a broad spectrum of projects involving risk assessment and process hazard analysis.
- Designed a heater treater unit to treat crude oil emulsions for XTO Energy which is a subsidiary of ExxonMobil.

**Undergraduate Research Assistant** in Chemical Engineering — Jan 2019 – Dec 2019
*Toley Lab, Indian Institute of Science, Bengaluru* — Karnataka, India

- Developed and published an algorithm to simulate Loop Mediated Isothermal Amplification (LAMP) of DNA.
- Modelled lateral flow bioreactions in sandwich assays.

## Publications and Conference Presentations

### Peer Reviewed Articles

[1] M. S. Priyadarshini, N. K. Thota, and R. Hernandez, "ReLMM:reinforcement learning optimizes feature selection in modeling materials", *Journal of Chemical Information and Modelling*, vol. 65, no. 1, pp. 153–161, 2025. DOI: 10.1021/acs.jcim.4c01934.

[2] N. K. Thota, M. S. Priyadarshini, and R. Hernandez, "NestedAE: Interpretable nested autoencoders for multi-scale material characterization", *Materials Horizons*, vol. 11, pp. 700–707, 2024. DOI: 10.1039/D3MH01484C.

[3] N. K. Thota, S. Quirk, Y. Zhuang, E. Stover, R. L. Lieberman, and R. Hernandez, "Correlation between chemical denaturation and the unfolding energetics of acanthamoeba actophorin", *Biophysical Journal*, vol. 122, pp. 2921–2937, 2022. DOI: 10.1016/j.bpj.2022.11.2941.

[4] Y. Zhuang, N. K. Thota, S. Quirk, and R. Hernandez, "Implementation of telescoping boxes in adaptive steered molecular dynamics (asmd)", *Journal of Chemical Theory and Computation*, vol. 18, pp. 4649–4659, 2022. DOI: 10.1021/acs.jctc.2c00498.

[5] N. Kaur, N. K. Thota, and B. J. Toley, "A stoichiometric and pseudo kinetic model of loop mediated isothermal amplification", *Computational and Structural Biotechnology Journal*, vol. 18, pp. 2336–2346, 2020. DOI: 10.1016/j.csbj.2020.08.020.

### Conference Presentations

[6] N. K. Thota, M. S. Priyadarshini, and R. Hernandez, *Multiscale modeling of materials using nested autoencoders*, Presented at AI-X Foundry Symposium, Johns Hopkins University, Baltimore, MD, USA, 2023.

[7] N. K. Thota, S. Quirk, Y. Zhuang, E. Stover, R. L. Lieberman, and R. Hernandez, *Mutational assay of an actophorin protein using adaptive steered molecular dynamics*, Presented at American Chemical Society Conference, Chicago, IL, USA, 2022.

## Teaching and Mentoring

- Instructor for Software Carpentry (EN.540.635). — Sep 2024 – Dec 2024
- Mentored a high school student on the basics of data analysis and machine learning in Python during my internship at PNNL. — Jul 2024 – Sep 2024
- Created content and taught a class on using PyTorch for Machine Learning in a Python Summer School led by Dr.Pratyush Tiwary. — Jul 2023 – Aug 2023
- Graduate Teaching Assistant for Process Dynamics and Control (EN.540.409.01). — Sep 2022 – Dec 2022

## Awards, Fellowships and Recognition

- Recipient of the 2022 Chemical and Biomolecular Engineering Committee for Diversity and Inclusion (CDI) Travel Grant for visiting the Fall 2022 American Chemical Society (ACS) Conference. Jun 2022
- Selected finalist among 30 candidates for Empower Your Pitch (EYP) competition. The competition is for Ph.D. students to communicate their research within 3 minutes to a non-specialist audience. Apr 2022
- Recipient of Chemical and Biomolecular Engineering Departmental Scholarship in the second year of my M.S.E. Sep 2021
- Gold medalist in Dr. P. K Karanth Memorial Quiz. An inter college quiz competition on the fundamentals of Chemical Engineering organized by the Indian Institute of Chemical Engineers (IIChE), Manipal Chapter. Special mention in IIChE 2018 Newsletter (Vol 10, Issue 4). Oct 2018

## Leadership

Department Representative in Graduate Representative Orgaization (GRO) Sep 2022 – Sep 2023
*GRO, Johns Hopkins University, Baltimore* Maryland, USA

- Represent the Graduate Students in the Chemical and Biomolecular Engineering Department for issues that pertain to all the graduate students at Johns Hopkins.

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

- Involved in organizing social and professional development events for graduate students in the Chemical and Biomolecular Engineering department.
- Organize student led seminars where we invite faculty from other universities to give talks in our department.
- Outside of college we enhance Johns Hopkins and the surrounding community through community service.

## Skills

- **Coding Languages:** Python, MATLAB, C++(basic proficiency)
- **Python Libraries:** Numpy, PyTorch
- **Languages:** Strong reading, writing and speaking competencies for English