

Nikhil Kumar Thota

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EDUCATION

Ph.D. in Chemical and Biomolecular Engineering <i>Johns Hopkins University, Baltimore</i>	Jan 2022 – Present Maryland, USA
M.S.E in Chemical and Biomolecular Engineering , GPA: 3.85/4.00 <i>Johns Hopkins University, Baltimore</i>	Sep 2020 – Dec 2021 Maryland, USA
B.Tech. in Chemical Engineering , GPA: 8.69/10.00 <i>Manipal Institute of Technology, Manipal</i>	Jul 2015 – May 2019 Karnataka, India

EMPLOYMENT HISTORY

Ph.D. Student in Chemical and Biomolecular Engineering <i>Hernandez Lab, Johns Hopkins University, Baltimore</i>	Jan 2022 – Present Maryland, USA
<ul style="list-style-type: none">– Ongoing thesis : “Data Driven Synthesis and Processing of Metal Halide Perovskites”– Developing Learning algorithms for multiscale modelling to learn how composition and synthesis conditions influence properties of Metal Halide Perovskites across different length scales.	
M.S.E Student in Chemical and Biomolecular Engineering <i>Hernandez Lab, Johns Hopkins University, Baltimore</i>	Sep 2020 – Dec 2021 Maryland, USA
<ul style="list-style-type: none">– Thesis: “Correlation Between Chemical Denaturation and the Unfolding Energetics of <i>Acanthamoeba Actophorin</i>”– 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 <i>Acanthamoeba Actophorin</i>.	
Process and Safety Engineer <i>ExxonMobil Services and Technology Private Limited, Bengaluru</i>	Jul 2019 – Aug 2020 Karnataka, India
<ul style="list-style-type: none">– 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 <i>Toley Lab, Indian Institute of Science, Bengaluru</i>	Jan 2019 – Dec 2019 Karnataka, India
<ul style="list-style-type: none">– 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. Thota, and R. Hernandez, “ReLMM: Reinforcement learning optimizes feature selection in material models”, in preparation.
- [2] N. Thota, M. S. Priyadarshini, and R. Hernandez, “NestedAE: Interpretable nested autoencoders for multi-scale material characterization”, 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

- 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. 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 (IChE), Manipal Chapter. Special mention in the IChE 2018 Newsletter (Vol 10, Issue 4). Oct 2018

LEADERSHIP

Department Representative in Graduate Representative Organization (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:** MATLAB, C++(basic proficiency), Python
- **Languages:** Strong reading, writing and speaking competencies for English