Subhadra Thapa, Ph.D.

subuthapa228@gmail.com
https://sites.google.com/view/biophysics-biochemistry LinkedIn
Google Scholar

Employment History

01/2025-present **Postdoctoral Research Associate,** Department of Physics, University of Vermont

4/2024-09/2024 **Postdoctoral Research Associate,** Department of Molecular Chemistry and molecular physiology, Purdue University

Education

2019 – 2024 **Ph.D., The Universty of Vermont** Material Science Specialization in Biomaterials
Thesis title: *Multiscale modeling to study the self/co-assembly of peptides*

2017 – 2019 **M.S. Physics, Biophysics** Theoretical Biophysics
Project title: *Computation of Meson mass.*

2007 – 2011 **B.S. Physics, Physics Major** Minor: Statistics and Math.

Research projects

Peptides aggregation — Multiscale modeling to study the self and co-assembly behaviour of peptides

Machine Learning — Prediction of Aggregation propensity of peptides using LSTM and Transfer Learning.

Drug Design — Ligand and structure based drug design.

Sensor Development — A generalizable fluorescence sensor platform for sample preparation-free protein detection.

Research Publications

Journal Articles

1. S. Thapa and J. Li, "Co-assembly of peptides and the role of hydrophobic residues in peptides co-assembly," *ACS Nano, submitted*, 2024.
2. S. Thapa and J. Li, "To aggregate, or not to aggregate, that is the question: Theoretical prediction and experimental validation of oligopeptide aggregation," *The Journal of Physical Chemistry Letters, To be submitted*, 2024.
3. H. Wu, T. Tuan, N. Tien, S. Thapa, J. Li, and T. Soh, "A generalizable fluorescence sensor platform for sample preparation-free protein detection," *Nature Communication, Under review*, 2024.
4. S. Thapa, F. clark, S. Scheneebeli, and J. Li, "Multiscale simulations to discover self-assembled oligopeptides: A benchmarking study," *Journal of chemical Theory and computation*, vol. 20, pp. 375–384, 2023.

Skills

Coding	Python, LaTeX
Data Science and ML	NumPy, Pandas, Jupyter-notebook, Matplotlib, Regression, Scikit-Learn, TensorFlow., etc.
Operating System	Linux, Mac OS, Windows
MD Simulation	GROMACS, DESMOND, CP2K
Enhanced Simulation	Metadynamics, Umbrella Samplings
CADD, Cheminformatics and others	Docking (GLIDE), Covalent Docking, WaterMap and SiteMap Prediction, Funnel Metadynamics
Visualization Software	VMD, PyMol, Maestro, UCSF Chimera, etc.
Structure Prediction	Alphafold, homology modeling
Teaching Experience	The University of Southern Mississippi, Undergraduate Physics lab (2017–2019), The Univesity of Vermont, Undergraduate Physics Lab (2019-2022)
Misc.	Academic research, teaching, training, Team leader, Under graduate and Graduate Mentoring, LaTeX typesetting and publishing.

Miscellaneous Experience

Certification

2022 **High-Throughput Virtual Screening for Hit Finding and Evaluation**.Awarded by Schrodinger.

2021 **Introduction to molecular modeling in drug discovery**.Awarded by Schrodinger.

References

Available on Request