Subhadra Thapa, PhD.

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🌐 https://sites.google.com/view/biophysics-biochemistry   in LinkedIn

Google Scholar

Employment History

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

4/2024-0 /2024   🔖 **Postdoctoral Research Associate**, Department of Molecular Chemistry and molecular physiology, Purdue University

Education

201 – 2024   🔖 **Ph.D., The Universty of Vermont** Material Science Specialization in Biomaterials
T esis title: *Multiscale modeling to study the self/co-assembly of peptides*

201 – 201   🔖 **M.S. Physics, Biophysics** T eoretical Biophysics
Project title: *Computation of Meson mass*

200 – 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 f uorescence sensor platform for sample preparation-free protein detection.

Research Publications

Journal Articles

1. S. T apa and J Li, "Co-assembly of peptides and the role of hydrophobic residues in peptides co-assembly," *ACS Nano, submitted*, 2024.

2. S. T apa and J Li, "To aggregate, or not to aggregate, that is the question: T eoretical prediction and experimental validation of oligopeptide aggregation," *T e Journal of Physical Chemistry Letters, To be submitted*, 2024.

3. H. Wu, T. Tuan, N. Tien, S. T apa, J Li, and T. Soh, "A generalizable f uorescence sensor platform for sample preparation-free protein detection," *Nature Communication, Under review*, 2024.

4. S. T apa, F. clark, S. Scheneebeli, and J Li, "Multiscale simulations to discover self-assembled oligopeptides: A benchmarking study," *Journal of chemical T eory and computation*, vol. 20, pp. 3 5-3 4, 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 (201 –201), The Univesity of Vermont, Undergraduate Physics Lab (201 -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 anddi** ▢