ROSHAN SHRESTHA

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EDUCATION

Modeling Bioglical Macromolecules team	*7 passage du Vercors, 69367 LYON Cedex 07*
Molecular Microbiology and Structural Biochemistry (MMSB)	2021 - Present

PhD in Computational Biophysics (Defense scheduled: September 23, 2025)
Institut de Biologie et Chimie des Protéines (IBCP)

Tribhuvan University	*Kirtipur, Kathmandu*
Master's Degree in Science (Physics)	2019
Central Department of Physics	CGPA 3.48/4.0

Patan Multiple College	*Patan*
Bachelor's Degree in Science (Major in Physics)	2011
Tribhuvan University	

PROFESSIONAL SUMMARY

PhD candidate in Computational Biophysics with 7+ years of experience in molecular modeling, coarse-grained simulations (Martini), and scientific computing. Skilled in Python, GROMACS, and multiscale analysis of biomolecules and nanomaterials. Proven track record of international collaboration and high-impact publications. Currently seeking a research-driven role in industry where I can apply my expertise in molecular simulations, data analysis, and model development to real-world challenges in materials science or biotechnology.

KEY SKILLS (TECHNICAL HIGHLIGHTS)

- **Molecular Simulations:** GROMACS, OpenMM, NAMD
- **Enhanced Sampling:** Umbrella Sampling, Metadynamics
- **Programming:** Python, Fortran, Bash, TCL
- **Machine Learning:** scikit-learn, PyTorch (basic), Molecular ML applications
- **Data Analysis:** NumPy, Pandas, SQL
- **Visualization:** Matplotlib, Xmgrace, Gnuplot

RESEARCH EXPERIENCE

M.Sc. Researcher	2014 - 2016
Central Department of Physics, Tribhuvan University	*Kirtipur*

- Worked on both atomistic and coarse-grained molecular dynamics simulation of proteins in lipid bilayers.
- Acquired knowledge and skills in free energy calculations using both umbrella sampling and enhanced collective variable sampling method like metadynamics.
- Conducted data analysis using python, numpy, matplotlib and pandas.
- Presented my work at both national and international conferences.

Graduate Research Assistant 2017 - 2019

GCK's Computational Lab, Central Department of Physics, Tribhuvan University *Kirtipur*

- Assisted both Bachelor's and Master's students to run Ab initio calculations and Molecular Dynamics Simulations.

- Defended thesis on **"A MOLECULAR DYNAMICS STUDY IN STRUCTURAL DYNAMICS OF A V717I SUBSTITUTION IN THE AMYLOID PRECURSOR PROTEIN"** to a jury of thesis committee.

- Currently working on **A Molecular Dynamics Study of Nanoparticle Interactions with Glycophorin - A** in collaboration with Dr.Anthony Nash and Dr. Sang Young Noh.

AWARDS/HONORS

- Awarded for the best poster by American Chemical Society (ACS) during ICAN-2019 held at ABV-IIITM, Gwalior, India, on 27-29 Jan, 2019

- Won the best poster by BioExcel at the BioExcel Winter School on Biomolecular Simulations, on 30th Nov - 4 Dec, 2020

- Won the best poster on " "Adsorption of Albumin on Graphene and Graphene Oxide: insight from molecular simulations" at NanoTox 2024

SELECTED PUBLICATIONS

- Naz Z, Shrestha R, et al. *Interaction of Phthalates with Lipid Bilayers.* J. Phys. Chem. B, 2022.

- Shrestha R, et al. *Martini 3 coarse-grained models for Carbon Nanomaterials.* ChemRxiv, 2024.

- Cambiaso S, Shrestha R, et al. *Martini 3 coarse-grained model for chitosan with tunanble acetylation.* ChemRxiv, 2025.

LANGUAGES

English: Professional proficiency
French: A1, actively learning
Dutch: A1, actively learning

CERTIFICATIONS

Python for Data Science Tips, Tricks, & Techniques — LinkedIn Learning
Learn Data Analysis with Pandas — Codecademy
Python Statistics Essential Training — LinkedIn Learning
Learn Git — Codecademy
Learning Bash Scripting — LinkedIn Learning
Functional Programming with Python — LinkedIn Learning
Additional: Linux CLI, Markdown, Object-Oriented Python, Web Scraping, NumPy/Statistics