

ROSHAN SHRESTHA

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EDUCATION

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

OBJECTIVE

I am a PhD student specializing in Computational Biophysics with a focus on computational modeling of biological systems and nanomaterials. I want to leverage my training in biophysics to further enhance my skills in modeling complex biological systems and nanomaterials, contributing to advancements in the field.

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-IITM, 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

TRAINER

Central Department of Physics

Tutor

Kirtipur

14-15 May, 2016

- Contributed the hands-on session as a tutor in training program on Computational Physics supported by UGC, Nepal, IEEE Nepal Chapter and ICTP Trieste, Italy.

Patan Multiple Campus

Trainer

Patan

8-10 June, 2017

- Trained M.Sc (Physics) students of Patan Multiple Campus during three days workshop on Fortran and Gnuplot.

INVITED TALK

Patan Multiple Campus

Guest Presenter

Patan

February, 2017

”Introduction to molecular visualization using VMD”

TEACHING EXPERIENCE

Rashmi Secondary School

Secondary School Science Teacher

Swoyambhu, Kathmandu

August 2011 - February 2014

- Taught Science to secondary level Science students (Grade 9 and 10) and supervise their laboratory works.

Ed Mark Academy

High School Physics Teacher

Kalanki, Kathmandu

October 2018 - March 2019

- Prepared and delivered lectures to high school physics students and supervise their laboratory works.

Bright Future Secondary School

High School Physics Teacher

Naikap, Kathmandu

April 2019 - July 2021

- Prepare and deliver lectures to high school physics students and supervise their laboratory works.

OTHER EXPERIENCE

- Organized Biophysics Week 2018 at Chelsea International College and Biophysics Week 2019 at Siddhartha Multiple College, Kathmandu in order to raise awareness of the field of biophysics among young high school students.
- As an overleaf advisor, conducted workshop on the use and power of LaTeX to local scientific community.

PROFESSIONAL MEMBERSHIP

- Member, Nepal Physical Society

SKILLS & INTERESTS

Programming: Python, Fortran, Bash Scripting, TCL Scripting
Software & Tools: MS Office, Latex, VMD, Adobe Illustrator, GROMACS, NAMD, Numpy, Pandas, Numpy, Matplotlib, Gnuplot, Grace
Interests: Graphics Design, Trekking, Hiking

PUBLICATIONS

- Naz, Z., Shrestha, R., Moin, S. T., & Monticelli, L. (2022). Interaction of Phthalates with Lipid Bilayer Membranes. *The Journal of Physical Chemistry B*, 126(25), 4679-4688

PUBLICATIONS (IN PREPARATION)

- Shrestha, R., Alessandri, R., Vögele, M., de Souza, P. C. T., Marrink, S., J., & Monticelli, L. Martini Coarse-Grained Models for Carbon Nanoparticles
- Shrestha, R., Hilpert, C., Cambiaso, S., Bochicchio, D., Rossi G., & Monticelli, L. Martini Coarse-Grained Model for Graphene oxide
- Cambiaso, S., Bochicchio, D., Shrestha, R., Rossi, & Monticelli, L. Martini 3 coarse-grained model for chitosan with tunable acetylation
- Crespi Veronica, Shrestha, R., di Meo F., & Monticelli, L. Simulating membrane proteins in asymmetric membranes.