

Prabin Baral

Academic Address: Department of Pharmaceutical Sciences, 20 Penn Street, Room 629 Baltimore, MD 21201

E-mail: prbnbaral@gmail.com, **cell:** +1-786-585-3365

LinkedIn: <https://np.linkedin.com/in/prabin-baral-490080116>

Objectives

To take up a challenging job in R & D position and contribute through my hard work, perseverance, sincerity and dedication for the growth of organization as well as myself as a promising professional.

Education and Affiliation

Postdoctoral Scholar *School of Pharmacy, University of Maryland, Baltimore*
MacKerell Lab *May 2022 - Present*
Force Field development of the CHARMM additive and Drude Polarizable force fields for biologically relevant compounds including DNA/RNA;

Postdoctoral Scholar/NIH-T32 Trainee *August 2023 - Present*
Simulation and investigations of biological systems (proteins, nucleic acids, etc) at different physiological setup using additive as well as drude FF
PI: Alexander D. MacKerell Jr.

Ph.D. in Physics *Florida International University*
Computational Biophysics Program *August 2016 - May 2022*
Dissertation Title: In-Silico Identification of Vaccine Candidates Against Viral Infections
Advisors: Bernard S. Gerstman, Prem P. Chapagain

M.Sc. in Physics *Tribhuvan University*
Major: Solid State Physics *2012-2015*
Courses Taken: Mathematical Physics, Classical and Statistical Mechanics, Quantum Mechanics, Electrodynamics, Solid State Physics
Dissertation: First-Principles Studies of Adsorption of F2 and I2 Molecules on MoS2 Monolayer
Advisors: Narayan P. Adhikari, Nurapati Pantha

Skills & Expertise

CHARMM, NAMD, OpenMM, VMD, PyMOL, TCL, awk, BASH, Linux and UNIX OS, HPC/GPU and XSEDE-clusters, PYTHON, Perl, Quantum Espresso

Research/Teaching Experiences

Computer Aided Drug Design Center (CADD) *May 2022 - Present*
Postdoctoral Scholar/NIH-T32 Trainee *Baltimore, US*

- Applied machine learning techniques to optimize the existing drude polarizable force field for nucleic acids
- Optimization of Force Field parameters and investigations of DNA and RNA systems under different physiological conditions
- Exploring Temperature Dependent Conformational Changes in MAP Kinases

Florida International University *August 2016 - May 2022*
Graduate Teaching/Research Assistant *Miami, Florida*

- Mentored and Taught Undergraduate Physics (2048L/2049L) Labs
- Mentored and Taught Astronomy Labs: Both Descriptive (AST1002L) as well as Solar System Astronomy (AST2003L)

- System setup and simulations of various biological systems (proteins, lipids, membranes, nucleic acids, etc) and studies of protein-protein, protein-lipid-membrane interactions and structure function relationship
- Virtual screening of library of small molecules against the therapeutic targets
- Collaborated with several cross departmental research subgroups, experimental laboratories as well as industrial partners with successful project coordination that resulted in several publications
- Won the Prestigious Dissertation Year Fellowship (DYF) award for demonstration of excellence in the research projects
- Travel allowances for conference presentations for four consecutive years (2018-2022): Awarded by College of Arts, Sciences and Education (CASE) as well as Graduate and Professional Student Committee (GPSC), FIU

Tribhuvan University

MS student

July 2012 - August 2016

Kathmandu, Nepal

- Investigated the adsorption of different halogens on MoS₂ monolayer by using density functional theory to investigate their bands, DOS, structural stability, etc.

Rising Rays Secondary School

Instructor

December 2015 - March 2016

Kathmandu, Nepal

- Competencies: Developing the assignments, exam and quizzes, conducting exams, grading, interaction with the parents about the progress in class

Publications & Presentations

Manuscripts Published (peer reviewed): 16

International Conferences Participated and Presented: 6

Extracurricular activities

Editor

2015

-Symmetry, Annual Scientific Magazine published by Central Department of Physics, Tribhuvan University, Nepal.

Treasurer

January 2018-January 2019

Nepalese Students Association, FIU (NSA@FIU)

Miami, Florida

Represented Nepal in the University and conducted several cultural activities and organized the national festival, blood drive programs together with the red cross society, etc.

Language proficiencies

English Read, Write, Speak

Nepali Read, Write, Speak

Hindi Read, Write, Speak

Memberships

Biophysical Society (BPS)

American Physical Society (APS)

American Chemical Society (ACS)