MAHESH KUMAR NEUPANE

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EDUCATION

St. Xavier's College, Maitighar, Nepal (Affiliated to **Tribhuvan University**) Sep 2024
Bachelor of Science in Physics Average percentage: 68.50 (CGPA: 3.54/4.00 Alpha Grade conversion)

PUBLICATIONS

1. Study on the Molecular Dynamics of 2-(4-fluorophenyl)-6-methyl-4-(3-(trifluoromethyl)phenyl)-1,2-dihydrodipyrazolo[3,4-b:3',4'-d]pyridin-3(6H)-one for Cancer Immunotherapy Using a DFT Model
***M. K. Neupane**, B. S. Magar, B. Gurung, R. R. Lamichhane, P. Pandey*
ACS Omega, Q1, 2025, DOI: link
Contribution: Performed DFT and MD simulations; calculated HOMO-LUMO, NBO, ELF, LOL, RDG; simulated FT-IR, Raman, UV-Vis; conducted molecular docking with CD28, CD80, CD86, CTLA-4; ADMET analysis; manuscript writing.

2. Comparative Study of Soft and Hard Boundary Constraints in Physics-Informed Neural Networks for Quantum Mechanical Eigenvalue Problems
A. Dhamala, S. Bhattarai, B. Gurung, C. Hyolmo, **M. K. Neupane**, R. R. Lamichhane, S. Chaulagain, B. S. Magar*
Heliyon, Q1, Submitted, 2025, DOI: link
Contribution: Developed PINN models; implemented soft and hard BCs; benchmarked against analytical/numerical solutions; adaptive learning rate optimization; evaluated efficiency and accuracy.

3. Theoretical Investigation on PD-L1-In-1 for Cancer Immunotherapy via Density Functional Theory
*B. Sijapati Magar, K. Pudasainee, P. Pandey, **M. K. Neupane**, et al.*
Scientific Reports, Q1, 2025, DOI: link
Contribution: DFT-based structural, electronic, and spectroscopic characterization; NBO analysis; HOMO-LUMO and DOS studies; molecular docking with PD-L1; predicted pharmacokinetics and biological activity.

RESEARCH EXPERIENCE

Independent Research Project july 2025 – Nov 2025
DFT Modeling & Molecular Docking for Cancer Immunotherapy
- Led a comprehensive *in silico* characterization of a novel small-molecule inhibitor targeting the B7-CD28 signaling axis for cancer immunotherapy application.
- Employed Density Functional Theory (DFT) at the B3LYP/6-311G(d) level using **Gaussian 09W** to simulate molecular geometry, electronic properties, and vibrational/NMR spectra.
- Conducted molecular docking simulations using **AutoDock Vina**, demonstrating strong binding affinity toward CTLA-4 (-7.97 kcal·mol^{-1}) and CD80 (-7.54 kcal·mol^{-1}) checkpoint proteins.
- Performed advanced topological analyses (ELF, LOL, RDG) and Natural Bond Orbital (NBO) analysis to visualize intermolecular interactions and electronic stability in polar solvents.
- Analyzed ADMET properties to predict favorable pharmacokinetics, confirming high human intestinal absorption (94%) and drug-likeness.
- Published results as the **Main Author** in *ACS Omega* (2025).

ML based Research Project Jun 2025 – Sep 2025
Boundary Constraints for Physics-Informed Neural Networks (PINNs)
- Initiated and coordinated a study with seven peers to investigate how boundary condition enforcement techniques affect solution accuracy and convergence in PINNs.
- Compared the performance of soft- and hard-constrained models in solving the Schrödinger equation for various potentials, benchmarking against analytical and numerical solutions.
- Demonstrated that hard-constrained models with ansätze reflecting the required asymptotic behavior and a variable parameter converge faster and achieve higher accuracy.
- Achieved over **100**× improvement in accuracy using adaptive learning rates for hard-constrained models compared to constant rates.

- Co-authored a manuscript detailing methodology and results.

ADDITIONAL PROJECTS

TargetScoreAI – AI Adaptive Learning Platform *2025*
targetscoreai.xyz | 2nd Place Asia-wide
- Developed platform serving 1,500+ users with adaptive algorithms.
- Built Python-React-PostgreSQL backend with analytics dashboards.
- Demonstrated ability to deliver production-grade AI systems.

SKILLS

Programming: Python (NumPy, Pandas, Matplotlib, PyTorch), C
Tools: Jupyter Notebook, Git, LaTeX, Gaussian 09W, VEDA 4, Multiwfn, GaussSum, AutoDock Vina
Languages: Nepali, English (**IELTS 7.0 overall**)

WORKSHOPS & TRAINING

- Trained in X-ray diffraction (XRD) methods for crystal structure determination and data interpretation, *Charotar University of Science and Technology (CHARUSAT), India* 2024
- Participated in a particle physics mini-workshop simulating Higgs boson data analysis, gaining experience in event-based data analysis and visualization, *ICTP Physics Without Frontiers* 2023
- Gained the experience of training neural networks on high-performance computing infrastructure for physics and engineering applications, *Kathmandu University (KU), Nepal* 2022

TEACHING EXPERIENCE

- Private Physics Tutor – Grade 12 Feb 2024– Sep 2024
  wave motion, electric circuits, intro to nuclear and particle physics
- NEB (Nepal Education Board) high school Math tutor Nov 2024 – Present
  complex numbers, counting problems, vectors, calculus, statistics

HONORS & AWARDS

- College Need-Based Scholarships (2020–2023).
- 2nd Place, Lovable Shipped Program for TargetScoreAI (Asia-wide).
- Recognition for Volunteer Work in Community Outreach Projects, Nepal.

LEADERSHIP & ACTIVITIES

- **Founder & Charter President, Leo Club of Kathmandu** (2020–2023) – Founded a 30-member chapter; led 12+ community and STEM outreach events; managed fundraising and logistics. [Link]
- **Volunteer, Be the Change Project** (2021–2022) – Established a library for underprivileged students in Sindhupalchowk; coordinated book collection and distribution. [Link]
- **Lead Demonstrator, Live Physics Expo (SXPC-Nepal)** (2024) – Organized interactive physics demonstration stalls for 200+ students. [Link]
- **Outreach Volunteer, IAPS School Day Programme** (2022) – Delivered physics demonstrations and STEM awareness sessions in rural schools. [Link]

REFERENCES

Available upon request.