ROSHAN SHRESTHA, PH.D.

Groefplein 6, Leuven 3000
(+32) 485 33 29 66 ◇ roshanpra@gmail.com ◇ roshan2004.github.io

PROFILE

Research Engineer and Computational Scientist with 7+ years of experience in molecular-scale and multi-scale simulations for advanced materials and biomolecular systems. Specialized in translating research-grade computational models into robust, reproducible, and industry-ready tools through workflow automation and model productization.

Currently working at **Materialise**, applying physics-based molecular modeling, data analysis, and scalable simulation pipelines to support industrial R&D, process understanding, and digital materials engineering.

TECHNICAL EXPERTISE

- **Molecular Simulation & Multiscale Modeling:** Coarse-grained (Martini 3) and atomistic MD; force-field development; free-energy methods (umbrella sampling, metadynamics).
  Tools: GROMACS, OpenMM, NAMD
- **Scientific Computing & Data Engineering:** Python (advanced), Bash, Fortran, TCL, SQL; reproducible workflows; HPC scripting; pipeline automation.
  Stack: NumPy, Pandas, Git
- **Machine Learning & Statistics:** Regression, classification, and feature engineering for materials and molecular property prediction.
  Frameworks: scikit-learn, PyTorch

PROFESSIONAL EXPERIENCE

Research Engineer *Sept 2025 – Present*
Materialise NV, Leuven, Belgium

- Integrate physics-based molecular simulations into industrial R&D workflows, supporting digital materials engineering, faster iteration cycles, and **data-driven decision-making**.
- Productize research-grade computational models into robust, reusable, and scalable engineering tools aligned with industrial constraints.
- Develop and validate standardized simulation workflows with strong emphasis on reproducibility, robustness, and model transferability.
- Collaborate with multidisciplinary teams to translate computational insights into actionable, product-oriented decisions.

PhD Researcher — Computational Biophysics *2021 – 2025*
Université Claude Bernard Lyon 1, France

- Developed and validated coarse-grained models (Martini 3) for carbon based nanomaterials for molecular dynamics simulations, reducing computational cost by orders of magnitude compared to atomistic methods while maintaining experimental accuracy.
- Built automated simulation and analysis pipelines (Python, Bash) to handle large-scale datasets with improved efficiency and reproducibility.

- Quantified critical interfacial thermodynamic properties using enhanced sampling (Metadynamics, Umbrella Sampling) to directly guide material design choices and optimize performance parameters.
- Delivered validated computational models resulting in multiple peer-reviewed ACS publications with demonstrated applied relevance.

SELECTED PUBLICATIONS

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

Shrestha, R., et al. *Martini 3 Coarse-Grained Models for Carbon Nanomaterials. J. Chem. Theory Comput.*, 2025.

Cambiaso, S., **Shrestha, R.**, et al. *Martini 3 Coarse-Grained Model for Chitosan with Tunable Acetylation. Biomacromolecules*, 2025.

EDUCATION

PhD in Computational Biophysics 2025
Université Claude Bernard Lyon 1, France

M.Sc. in Physics 2019
Tribhuvan University, Nepal

ADDITIONAL INFORMATION

Awards: Best Poster Awards — ACS ICAN 2019; BioExcel Winter School 2020; NanoTox 2024

Languages: English (Professional), French (A1), Dutch (A1)