Rahul Sheshanarayana

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scholar.google.com/citations?user=Zhd0xIMAAAAJ&hl=en&authuser=5

PhD researcher focused on designing safer molecules and remediating PFAS contamination. Developed generative models, scalable ML systems, and molecular simulation tools with demonstrated impact across sustainability and materials science. 7+ publications in leading journals including *Advanced Science*, *Nature Communications*, and *Digital Discovery*, with multiple journal covers and an Editor's Pick.

Education

PhD, Cornell University **Aug 2024 - Present**

Major - Systems Engineering

Thesis title: Thermochemistry-aware Machine Learning for Sustainable Molecular Design: Representation Learning, Radical Design, and PFAS Remediation

Thesis advisor: Dr. Fengqi You

MS, Cornell University **Aug 2022 - May 2024**

Major - Chemical Engineering

Thesis title: Probing Ion Effects In Nanoconfined Aqueous Electrolytes: A Molecular Dynamics Study Using Neural Network Potentials

Thesis advisor: Dr. Shuwen Yue

BTech, Indian Institute of Technology (IIT) Roorkee **Aug 2018 - May 2022**

Major - Polymer Science, Minor - Applied Mathematics

Thesis title: A Kinetic Model for the Direct Thermal Liquefaction of Pine Wood

Thesis advisor: Dr. Shushil Kumar

Research Experience

Department of Systems Engineering, Cornell University **Aug 2024 - Present**

- Designed a bond dissociation energy (BDE)-conditioned transformer for generative molecular design, achieving distributional control over radical bond strengths with 81-94% validity and 84-92% novelty across BDE targets.
- Achieved up to 90% R^2 improvement in molecular property prediction by distilling SchNet and DimeNet++ into 2× smaller student GNNs, across QM9, ESOL, and FreeSolv datasets.

Department of Chemical Engineering, Cornell University **Aug 2022 - July 2024**

- Trained DFT-accurate neural network potentials via active learning on HPC clusters for nanoconfined electrolytes, reaching force RMSEs $\leq$ 0.07 eV/Å and enabling fast MD simulations.
- Identified ion-specific interfacial behavior in confined electrolytes; K^+ showed 3× stronger adsorption and 2× faster diffusion than Na^+, trends absent in classical force fields.

Department of Chemical Engineering, IIT Roorkee **Aug 2021 - Aug 2022**

- Developed a kinetic model for pine wood liquefaction, finding distillate formation nearly 2× faster than heavy residue, with secondary reactions negligible.
- Demonstrated that adding 20 wt% water more than doubled primary reaction rates, with guaiacol:water = 8:1 giving the highest overall conversion.

Department of CSE, Jadavpur University **Jan 2021 - Aug 2022**

- Boosted vehicular smoke detection accuracy by up to 12% mAP across 3 public datasets using a λ-attention transformer head on a YOLOv5 backbone.
- Increased training coverage by 5× with a dual-level synthetic smoke generation pipeline (mask patterns + filtering) to overcome limited real-world data.

Department of Chemical Engineering, Indian Institute of Science **Nov 2020 - Apr 2022**

- Achieved 97% R^2 for nanopore formation probability and 95% R^2 for formation time prediction by training a two-stage ML framework on 20,840 unique graphene nanopore structures.
- Quantified the effect of 18 structural features (e.g., rim atoms, shape factor, symmetry) on pore formation kinetics using SHAP-based feature importance, providing interpretable physical insights.

Publications

Sheshanarayana, R., You, F. (2026). Harnessing homolytic bond energetics to steer inverse radical design. *Submitted.*

Sheshanarayana, R., You, F. (2025). Rethinking Retrosynthesis: Curriculum Learning Reshapes Transformer-Based Small-Molecule Reaction Prediction. *J. Chem. Inf. Model.*, 65(20), 11047-11063. ***Supplementary Journal Cover***.

Sheshanarayana, R., You, F. (2025). Molecular Representation Learning: Cross-domain Foundations and Future Frontiers. *Digital Discovery*, 2298. ***Journal Inside Front Cover***.

Sheshanarayana, R., You, F. (2025). Knowledge Distillation for Molecular Property Prediction: A Scalability Analysis. *Advanced Science*, 2503271. ***Journal Frontispiece***.

Verma, A.M., Chaturvedi, S., Paul, S., Nandi, S, **Sheshanarayana, R.**, Santhosh, K., Valavarasu, G., Dukkipati, A., Gwie, C.G., Moo, P.Y., Ng, C.Q.J., Amrute, A., Govind Rajan, A. (2025). Data-driven massive reaction networks reveal new pathways underlying catalytic CO2 hydrogenation. *Under review at Nature Communications*.

Sheshanarayana, R., Kumar, S. (2025). A kinetic model for the direct thermal liquefaction of pine wood. *Biomass Conversion and Biorefinery*, 15(17), 23795-23803.

Kundu, S., Maulik, U., **Sheshanarayana, R.**, Ghosh, S. (2022). Vehicle Smoke Synthesis and Attention-based Deep Approach for Vehicle Smoke Detection. *IEEE TIA*, 59(2), 2581-2589.

Sheshanarayana, R., Govind Rajan, A. (2022). Tailoring nanoporous graphene via machine learning: Predicting probabilities and formation times of arbitrary nanopore shapes. *J. Chem. Phys.*, 156(20). ***Editor's pick***.

Skills

Scientific domains	Thermochemistry, reaction modeling, polymer science, nanoporous materials, confined electrolytes, statistical mechanics, computational fluid dynamics, linear/non-linear programming, goal programming, control theory.
Computational tools	Density functional theory, Monte Carlo simulations, molecular dynamics simulations, statistical optimization, machine learning, deep learning.
Software	Python, R, DPGEN, DeepMD, Quantum Espresso, ORCA, LAMMPS, MATLAB, LaTeX, VESTA, VMD.
ML packages	PyTorch, PyTorch Geometric, Hugging Face Transformers, Scikit-learn, ASE, RDKit, Optuna, Weights & Biases, TensorFlow, Pandas, NumPy, Matplotlib.

Teaching

Graduate Teaching Assistant (Investigative Biology Lab) **Aug 2023 - May 2025**

Taught 35 undergraduates per semester in Investigative Biology (BIOG 1500) at Cornell, covering experimental design, hypothesis testing, and statistical analysis through hands-on labs.

Graduate Teaching Assistant (Fundamentals of Physics II Lab) **Feb 2023 - May 2023**

Guided students through lab experiments ranging in topics from electricity and magnetism to optics.

Academic Awards

Best Bachelor's Thesis Award **Aug 2022**

Received for developing a kinetic model for the direct thermal liquefaction of pine wood, later published in *Biomass Conversion and Biorefinery*.

Editor's Pick - Journal of Chemical Physics **Jan 2022**

Awarded for "Tailoring nanoporous graphene via machine learning: Predicting probabilities and formation times of arbitrary nanopore shapes"- selected as Editor's Pick in the *Journal of Chemical Physics*.