Vinamr Jain

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PhD Student, Cornell University

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Machine learning PhD student at Cornell working on decision-making under uncertainty: how should an agent act when it doesn't even know what it's supposed to do, or what the rules are? I build the whole stack behind each result, from simulation environments to training and evaluation pipelines to the algorithms. Four published papers, including NeurIPS 2026. Seeking a research internship for summer 2027.

Education

Cornell University 2024 – 2029 (expected)
PhD · Advisors: Sarah Dean and Alexander Terenin

Indian Institute of Technology Delhi 2020 – 2024
B.Tech, Engineering Physics · CGPA 8.96/10

Research

Bayesian Decision Making in Unknown Dynamics Ongoing
Supported by a Cornell Atkinson 2030 Fast Grant ($26,000).

- Algorithmic framework for autonomous systems like weather balloons and saildrones that must plan their path when they don't know what the underlying wind or ocean currents are. Paper in preparation.
- Built zermelo (github.com/VinamrJain/zermelo), an open-source Gymnasium-style simulation environment in JAX.

Thompson Sampling with Prior-fitted Diffusion Transformers NeurIPS 2026

- Black-box optimization of unknown functions, using a diffusion model that learns in context: pretrained on simulated functions, it proposes the next point to evaluate with no model fitting at test time.
- Designed function priors and built the training and evaluation harness: multi-GPU training, SLURM, Weights & Biases sweeps.

AI for Scientific Discovery 2022 – 2025
Cornell (Fengqi You), Penn State (Romit Maulik), University of Exeter (Oleksandr Kyriienko).

- Three first-author papers: generative design of peptides that bind to microplastics, sea-surface-temperature forecasting with quantum reservoir computing, and a review of machine learning for battery materials.

Publications

Thompson Sampling using Prior-fitted Diffusion Transformers
Sihwa Park, Jingsen Zhu, **Vinamr Jain**, Sheng-Yen Chou, Alexander Terenin. *NeurIPS*, 2026

Machine Learning Pipelines for the Design of Solid-State Electrolytes
Vinamr Jain, Z. Wang, F. You. *Materials Horizons*, 2026

Higher-Order Quantum Reservoir Computing for Non-Intrusive Reduced-Order Models
Vinamr Jain, R. Maulik. *AIAA SciTech Forum*, 2026

AI-Driven Rational Design of Promiscuous and Selective Plastic-Binding Peptides
Vinamr Jain, M. T. Bergman, C. K. Hall, F. You. *Chemical Science, 16, 20823–20832*, 2025

Technical Skills

Machine learning: Reinforcement learning, Bayesian optimization, diffusion models, transformers, in-context learning, decision-making under uncertainty

Engineering: Python, C++, PyTorch, JAX, Weights & Biases, Docker, Git

Awards & Mentoring

NSF Research Traineeship (NRT) Award: AI for Science Program, Cornell University – $5,000 in GPU compute credits

Research Mentor · Bowers Undergraduate Research Experience, Cornell: two undergraduates · Summer 2026