

## Education

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- **Mila and Polytechnique Montréal**, Montréal, Canada *Aug'22-Present*  
PhD in Computer Engineering; Advisor: [Sarath Chandar](#)
- **Indian Institute of Technology Madras**, Chennai, India *Jul'17-Jul'22*  
Bachelor of Science in Biological Sciences and Master of Technology in Data Science  
Minor: Computational Biology *CGPA: 9.31/10.00*

## Research Experience

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- **Reinforcement learning for LLMs** *Sep'25-Present*  
Mentors: [Sarath Chandar](#), [Mathieu Reymond](#)
  - Currently working on improving exploration with intrinsic rewards in reinforcement learning-based fine-tuning of LLMs
- **AI-automated CAD object generation** *Jun'24-Present*  
Mentors: [Sarath Chandar](#), [Jay Pathak](#), [Quentin Fournier](#)
  - Collaboration with Ansys: LLMs for automated generation of 3D Computer-Aided Design (CAD) objects
  - Published CADmium, an open-source dataset and LLM fine-tuning approach [[Paper](#), [Code](#), [Website](#)]
- **Reinforcement learning for material design** *Aug'22-Present*  
Mentors: [Sarath Chandar](#), [Mathieu Reymond](#), [Santiago Miret](#), [Mariano Phielipp](#)
  - Project with Intel on offline and online reinforcement learning approaches for generating new crystal structures
  - Integrated first-principles density functional theory with conservative Q-learning – accepted at [MoML 2023](#), [A4Mat](#) workshop at [NeurIPS 2023](#), and [Digital Discovery](#) Journal [[Paper](#), [Code](#)]
  - Released CrystalGym, the first online RL environment and benchmark for material discovery – Spotlight at [A4Mat-ICLR 2025](#) [[Paper](#), [Code](#)]
- **Master's Thesis: Graph generative models for binding site-specific molecule generation** *Aug'21-Jun'22*  
Guides: [Balaraman Ravindran](#), [Karthik Raman](#), IIT Madras [[Thesis](#), [Poster](#)]
  - Designed graph variational autoencoder models for generation of drug molecules that can bind to a given binding site
  - Explored sequential models like RNN and LSTM for node and edge generation, and determined ways to mitigate order dependence during training
- **Analysis of drug response and gene expression data of AML cells** *Jun-Sep'21*  
Guide: [Brian Wilhelm](#), Université de Montréal (Virtual)
  - Performed analysis of drug response and gene expression data, focusing on Acute Myeloid Leukemia
  - Computational methods to identify drug-gene correlations and molecules that can induce leukemic cell maturation
- **Deep generative models for single-cell gene expression analysis** *May-Jul'20*  
Guide: [Hongyu Zhao](#), Yale University (Virtual)
  - Evaluated state-of-the-art unsupervised deep learning techniques including variational autoencoders for single-cell gene expression data analysis
- **RNA-seq data analysis of human oral squamous cell carcinoma** *May-Jul'19*  
Guide: [Debnath Pal](#), Indian Institute of Science Bangalore
  - Identified somatic mutations in RNA-sequencing data of human oral squamous cell carcinoma samples

## Projects

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- **Effects of visual representation for navigation control tasks** *Jan-Apr'23*  
Robot Learning, Université de Montréal
  - Studied effects of contrastive learning and VAE-based pretraining strategies for RL-based visual navigation
- **Incorporating geometry into score-based model for crystal structure design** *Sep-Dec'22*  
Geometry and Generative Models, McGill University
  - Attempted ways to incorporate crystal symmetry as an inductive bias into generative models for crystal structure design
- **Generating drug-like molecules from gene expression signatures using transformer** *Sep-Dec'20*  
Algorithmic Approaches to Computational Biology, IIT Madras [[Poster](#), [Video](#), [Report](#)]
  - Designed an attention-based transformer model for *de novo* generation of drug-like molecules that can induce a desired transcriptomic profile. Accepted as poster at [MLCSB COSI](#), [ISMB 2022](#)
  - Generated chemical compounds that were unique, valid, relevant, synthesizable and similar to known compounds
- **Parallel analyses of canonic polyadic tensor decomposition algorithm** *Feb-Jun'21*  
Parallel Scientific Computing, IIT Madras [[Report](#), [Code](#)]
  - CPU- and GPU-level parallelization of tensor decomposition algorithm using OpenMP and OpenACC
- **Deep generative approach to model single-cell data of human embryoid bodies** *Jan'20-Jul'20*  
Computational Systems Biology, IIT Madras
  - Worked on using deep generative variational autoencoder model (scVI) to identify biologically relevant cell types of single-cell human embryoid bodies

## Awards

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- **PBEEE** – Merit scholarship for international students awarded by Fonds de recherche du Québec
- **Khorana Program for Scholars 2020<sup>1</sup>** – Awarded by Department of Biotechnology, Government of India
- **INSPIRE Scholar** – Awarded by Department of Science and Technology, Government of India

## Publications ([Google Scholar](#))

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- Woo, Kowen\*, **Prashant Govindarajan\***, and Sarath Chandar. **“Benchmarking Machine Learning Potentials for Crystal Structure Relaxation.”** In NeurIPS 2025 AI for Science Workshop.
- **Govindarajan, Prashant**, Davide Baldelli, Jay Pathak, Quentin Fournier, and Sarath Chandar. **“CADmium: Fine-Tuning Code Language Models for Text-Driven Sequential CAD Design.”** arXiv preprint arXiv:2507.09792 (2025).
- **Govindarajan, Prashant**, Mathieu Reymond, Antoine Clavaud, Mariano Phielipp, Santiago Miret, and Sarath Chandar. **“CrystalGym: A New Benchmark for Materials Discovery Using Reinforcement Learning.”** arXiv preprint arXiv:2509.23156 (2025).
- **Govindarajan, Prashant**, Mathieu Reymond, Santiago Miret, Mariano Phielipp, and Sarath Chandar. **“Crystal Design Amidst Noisy DFT Signals: A Reinforcement Learning Approach.”** In AI for Accelerated Materials Design-NeurIPS 2024.
- **Govindarajan, Prashant**, Mathieu Reymond, Santiago Miret, Antoine Clavaud, Mariano Phielipp, and Sarath Chandar. **“A Reinforcement Learning Pipeline for Band Gap-directed Crystal Generation.”** In AI for Accelerated Materials Design-Vienna 2024.
- **Govindarajan, Prashant**, Santiago Miret, Jarrid Rector-Brooks, Mariano Phielipp, Janarthanan Rajendran, and Sarath Chandar. **“Learning Conditional Policies for Crystal Design Using Offline Reinforcement Learning.”** Digital Discovery (2024).
- **Govindarajan, Prashant**, Santiago Miret, Jarrid Rector-Brooks, Mariano Phielipp, Janarthanan Rajendran, and Sarath Chandar. **“Behavioral Cloning for Crystal Design.”** In Workshop on “*Machine Learning for Materials*” *ICLR 2023*. 2023.

**Accepted Posters:** [AI4Mat](#) workshop (ICLR 2025, Vienna 2024, NeurIPS 2023 & 2024), ML4Materials workshop at ICLR 2023, Molecular Machine Learning Conference ([MoML 2023](#) at MIT), Intelligent Systems for Molecular Biology ([ISMB 2022](#))

## Research Areas and Interests

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Reinforcement Learning, Large Language Models, AI-based Drug and Material Design, Geometric Deep Learning, and Computational Biology

## Relevant Coursework & Skills

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### Courses

Geometry and Generative Models, Reinforcement Learning, Representation Learning, Robot Learning, Parameter and State Estimation, Parallel Scientific Computing, Algorithmic Approaches to Computational Biology, Pattern Recognition and Machine Learning

### Skills

Python (PyTorch, Tensorflow), R, MATLAB, C/C++ (OpenMP, MPI, OpenACC), Matter Modeling (DFT)

## Activities & Extra-curriculars

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### Teaching

- [Machine Learning](#), Polytechnique Montréal, Fall 2025
- [Reinforcement Learning](#), Polytechnique Montréal, Fall 2023
- [Reinforcement Learning](#), IIT Madras, Spring 2022
- [DSA for Biology](#), IIT Madras, Fall 2021

### Activities

- Organizer of “AI for Materials” reading group at Mila.
- Instructor for Chandar Lab’s High School Internship Program
- Volunteer for [Graduate Application Assistance Program for Underrepresented Students in AI](#)
- Social events organizer at [Chandar Research Lab](#)
- Organizer of Molecular ML Conference ([MoML 2023](#) and [MoML 2024](#) at Mila)

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<sup>1</sup>Fellowship awarded to biotechnology students to undertake research internship in the USA [[Link](#)]

- Talk on “Deep Learning in Genomics and Drug Discovery”, IIT Madras
- Volunteered to anchor in [High Performance Computing Symposium](#), IIT Madras
- Former student member at the [New York Academy of Sciences](#) (NYAS)
- Reviewing**
  - [TMLR](#) (2025)
  - [AI4Mat](#) workshop (Vienna 2024, NeurIPS 2023 & 2024)
  - [MoML](#) (2023-25)
  - [Deployable AI](#) workshop (AAAI 2023)
- Competitions**
  - First prize in start-up pitch competition at [Sciencepreneurship](#), EPFL, Switzerland
  - Winning team, [MIT COVID-19 Challenge](#) (wastewater biosensor to track COVID-19)
  - Finalist, [Tracking Coronavirus Challenge](#) organized by NYAS
- Sports**
  - Ultimate Frisbee under National Sports Organization scheme at IIT Madras
- Others**
  - Summer Schools: [Oxford ML](#) (2024)<sup>2</sup>, [Sciencepreneurship](#) (2024), [Amii AI Week](#) (2022)
  - Coordinator, Sponsorship and Public Relations team, Shaastra<sup>3</sup> 2019, IIT Madras
  - Coordinator, Analytics Club, Center For Innovation<sup>4</sup>, IIT Madras

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<sup>2</sup>Declined

<sup>3</sup>Annual technical fest of IIT Madras

<sup>4</sup>Student-run innovation lab of IIT Madras