

# Vignesh Ram Somnath





✉ [vsomnath@ethz.ch](mailto:vsomnath@ethz.ch)

🐦 [@vsomnath](https://twitter.com/evsomnath)




🌐 [vsomnath.github.io](https://vsomnath.github.io)

📄 [vsomnath](#)

## Education

- 2021 – Now  **Eidgenössische Technische Hochschule (ETH) Zürich** *Zurich, Switzerland*  
PH.D IN COMPUTER SCIENCE (D-INFK)  
Thesis Advisors: Andreas Krause and Kjell Jorner  
Topic: *Geometric diffusion models with applications in structural biology and chemistry.*
- 2019 – 2020  **Massachusetts Institute of Technology (MIT)** *Cambridge, USA*  
VISITING STUDENT IN COMPUTER SCIENCE & CHEMICAL ENGINEERING  
Advisors: Regina Barzilay and Klavs Jensen
- 2017 – 2020  **Eidgenössische Technische Hochschule (ETH) Zürich** *Zurich, Switzerland*  
M.Sc. COMPUTATIONAL BIOLOGY AND BIOINFORMATICS  
Thesis Advisors: Andreas Krause (ETH), Regina Barzilay (MIT)
- 2013 – 2017  **Indian Institute of Technology (IIT) Madras** *Chennai, India*  
B. TECH. CHEMICAL ENGINEERING






## Research and Work Experience

- Fall 2023  **Student Researcher**, [GOOGLE DEEPMIND](#) *Zurich, Switzerland*  
Worked on protein representation learning with large language models (LLMs).
- 2020 – 2021  **Research Assistant**, [LEARNING & ADAPTIVE SYSTEMS](#) *Zurich, Switzerland*  
Developed a multi-scale graph model for representation learning on proteins.  
[Work](#) accepted to NeurIPS 2021.
- Summer 2019  **Student Developer**, [GOOGLE SUMMER OF CODE](#), [DEEPCHEM](#) *Zurich, Switzerland*  
Added support for transfer learning into DEEPCHEM. [GSoc Report](#) & [GitHub](#).



## Publications

\* denotes equal contribution.

### Conference and Journal Publications

- 2023  **Aligned Diffusion Schrödinger Bridges.**  
V. R. Somnath\*, M. Pariset\*, Y. Hsieh, M. R. Martinez, A. Krause, C. Bunne [UAI](#)
-  **Isotropic Gaussian Processes on Finite Spaces of Graphs.**  
V. Borovitskiy\*, M. R. Karimi\*, V. R. Somnath\*, A. Krause. [AISTATS](#)
- 2021  **Multi-Scale Representation Learning on Proteins.**  
V. R. Somnath\*, C. Bunne\*, A. Krause. [NeurIPS](#)
-  **Learning Graph Models for Retrosynthesis Prediction.**  
V. R. Somnath, C. Bunne, C. W. Coley, A. Krause, R. Barzilay. [NeurIPS](#)  
[Best Paper Award, ICML 2020 GRL+ Workshop](#)
-  **Mixture-of-Experts VAE for single-cell data generation.**  
A. Kopf, V. Fortuin, V. R. Somnath, M. Claassen. [PLOS Computational Biology](#)

### Preprints and Under Review

- 2023  **DockGame: Cooperative Games for Multimeric Rigid Protein Docking.**  
V. R. Somnath\*, P. G. Sessa\*, M. R. Martinez, A. Krause. [arXiv](#)
- 2022  **ChromFormer: 3D genome structure prediction using Transformers.**  
H. Valeyre, P. Pati, F. Gossi, V.R. Somnath, A.L. Martinelli, M. Rapsomaniki. [bioRxiv](#)

## Fellowships and Awards

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- 2020 **Best Paper Award**, ICML Workshop on Graph Representation Learning and Beyond
- 2019 **Master Thesis Grant**, Zeno Karl Schindler Foundation  
USD 12000 awarded in support for my Master Thesis at MIT
- 2018 **Birkigt Scholarship**, ETH Zürich  
USD 10000 awarded in support for my Master Studies at ETH

## Presentations

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### Conference and Workshop Talks

- 08/2023 **Spotlight Presentation**, Aligned Diffusion Schrödinger Bridges.  
UAI 2023 *Pittsburgh, USA*
- 07/2021 **Contributed Talk**, Multi-Scale Representation Learning on Proteins.  
ICML Workshop Computational on Biology *virtual*
- 07/2020 **Contributed Talk**, Learning Graph Models for Template-Free Retrosynthesis.  
ICML Workshop on Graph Representation Learning and Beyond *virtual*

### Seminars at Universities

- 09/2023 **Invited Talk**, DockGame: A Game-Theoretic Framework for Multimeric Docking.  
Data & ML Lunch Seminar, D-CHAB, ETH Zürich *Zurich, Switzerland*
- 03/2023 **Invited Talk**, Structural Priors for Learning Transformations in Chemical Processes  
NCCR Catalysis Annual Meeting *Luzern, Switzerland*

## Teaching

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- Fall 2023 **Teaching Assistant**, Probabilistic Artificial Intelligence
- Spring 2023 **Teaching Assistant**, Introduction to Machine Learning
- Fall 2022 **Teaching Assistant**, Probabilistic Artificial Intelligence
- Spring 2022 **Teaching Assistant**, Introduction to Machine Learning
- Fall 2021 **Teaching Assistant**, Probabilistic Artificial Intelligence

## Supervision

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- 2023 - now **Gabriel Cathoud**, Master Student, University of Coimbra  
Co-supervision with Kenza Amara and Kjell Jorner (ETH AI Center)
- Vishnu Nair**, Master Student, Adaptyv Bio  
Co-supervision with Daniel Gutierrez (Adaptyv Bio)
- 2022 **Henry Valeyre**, Master Student, ETH and IBM Research Zürich  
Co-supervision with Pushpak Pati and Marianna Rapsomaniki (IBM Research Zürich)
- 2021 **Teodora Bujaroska**, Master Student, ETH  
Co-supervision with Giuseppe Russo (ETH)

## Languages and Skills

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- Languages **English, Hindi, Tamil: Native Fluency**
- Coding **Python, R, Git,  $\LaTeX$**
- Libraries **PyTorch, TensorFlow, scikit-learn**