Charlotte Bunne

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Academic Positions

EPFL School of Computer and Communication Sciences and School of Life Sciences *Lausanne, Switzerland*
TENURE-TRACK ASSISTANT PROFESSOR *since fall 2024*
Group: Artificial Intelligence in Molecular Medicine

Stanford University and Genentech *San Francisco, USA*
POSTDOCTORAL RESEARCHER *2023 - 2024*
Advisors: Aviv Regev and Jure Leskovec

Education

Eidgenössische Technische Hochschule (ETH) Zurich *Zurich, Switzerland*
PHD IN COMPUTER SCIENCE *2019 - 2023*
- Doctoral Committee: Andreas Krause, Marco Cuturi, Lucas Pelkmans, and Jure Leskovec
- **ETH Medal** for best PhD thesis

Massachusetts Institute of Technology (MIT) *Cambridge, USA*
VISITING STUDENT IN COMPUTER SCIENCE *2018*
- Advisors: Stefanie Jegelka and David Alvarez-Melis

Eidgenössische Technische Hochschule (ETH) Zurich *Zurich, Switzerland*
M.S. IN COMPUTATIONAL BIOLOGY AND BIOINFORMATICS *2016 - 2019*
- **ETH Medal** for best Master thesis (awarded to top 2.5% of all ETH graduates)
- **Willi-Studer Prize** for best GPA and graduated with distinction
- Selected into the **Excellence Scholarship & Opportunity Program** (ESOP)

Heidelberg University *Heidelberg, Germany*
B.S. IN BIOSCIENCES *2013 - 2016*
- Major in Bioinformatics and graduated among top 2% of class
- Selected as Fellow of the **German Academic Scholarship Foundation** (Studienstiftung d. dt. Volkes)

Research and Work Experience

2022 - 2023	**Broad Institute of MIT and Harvard**, Graduate Researcher	Cambridge, USA
	• Supervisors: Anne Carpenter and Shantanu Singh	
2022	**Apple**, Research Intern	Paris, France
	• Machine Learning Group of Samy Bengio and Marco Cuturi	
2020	**Google Research**, Research Intern	Zurich, Switzerland
	• Brain Team of Jean-Philippe Vert and Marco Cuturi	
2019 - 2023	**ETH AI Center**, Graduate Researcher	Zurich, Switzerland
	• Supervisor: Andreas Krause	
2018	**MIT CSAIL**, Research Assistant	Cambridge, USA
	• Supervisors: Stefanie Jegelka and David Alvarez-Melis	
2017 - 2018	**IBM Research**, Software Engineering Intern	Zurich, Switzerland
	• Cognitive Computing and Industry Solutions Group of Maria Gabrani	
2015 - 2016	**German Cancer Research Center (DKFZ)**, Research Assistant	Heidelberg, Germany
	• Supervisors: Roland Eils and Thomas Höfer	

Fellowships and Awards

SELECTED AWARDS

2024	**ETH Medal**, ETH Zurich	*Best PhD Thesis in CS*
2024	**Best Paper Award**, ICML AI for Science Workshop	*1/148 Papers*
2024	**SIB Remarkable Outputs 2023 Award**, SIB Swiss Institute of Bioinformatics	

2024	**Finalist of the German Thesis Award**, Körber Stiftung	*11/719 Theses*
2021	**Best Paper Award**, ICML Time Series Workshop	*1/35 Papers*
2020	**Best Paper Award**, ICML Workshop on Graph Representation Learning & Beyond	*1/73 Papers*
2019	**ETH Medal**, ETH Zurich	*Top 2.5% of All ETH Graduates*
	Willi Studer Prize, ETH Zurich	*Best GPA of Cohort*
2018	**Best Paper Award**, NeurIPS Workshop on Relational Representation Learning	*1/52 Papers*
2014	**Grand Prize**, iGEM Competition	*1/245 Teams, 3 Special Prizes*
2012	**Grand Prize**, iGEM High School Competition	*1/40 Teams, 5 Special Prizes*

SELECTED FELLOWSHIPS

2020 **Generation Google Scholarship**, Google
Scholarship of $ 7000 and recognition for PhD studies.

2018 **Master Thesis Grant**, Zeno Karl Schindler Foundation
12,000 $ awarded in support for my Master thesis.
Fellowship for Graduate Studies Abroad, Dr. Jürgen Ulderup Scholarship
Academic scholarship in support for graduate studies abroad.

2016 - 2019 **Excellence Scholarship and Opportunity Award**, ETH Zurich
Excellence scholarship of the ETH Foundation covering the full study and living costs, i.e., ∼35,000 $.

2016 - 2019 **Fellow of German Academic Scholarship Foundation**, Studienstiftung d. dt. Volkes
Germany's *most prestigious* academic scholarship throughout my undergraduate and graduate studies.

2015 - 2017 **STEM Excellence Award**, Manfred Lautenschläger Stiftung
Scholarship of 3000 $ and recognition for Bachelor studies.

2010 - 2013 **Fellowship for Gifted Student**, Life Science Lab of the German Cancer Research Center
Science education of mathematically, scientifically, and technically particularly gifted high school students.

HONORS

2022 **Participant of Heidelberg Laureate Forum**, ETH Representative Heidelberg, Germany
Recipient of Rhein-Neckar Grant
Competitive selection of participating researchers in math and computer science.

2020 **Participant of Global Young Scientists Summit**, ETH Representative Singapore, SG
Competitive selection of participating young researchers in science, mathematics, and technology.

Press and Outreach

2025	**Ground Truths by Eric Topol**, "The AI virtual cell: the holy grail of biology."	
2025	**Nature**, "Self-driving labs, advanced immunotherapies and five more technologies to watch in 2025."	
2025	**The Atlantic**, "A Virtual Cell Is a 'Holy Grail' of Science. It's Getting Closer."	
2023	**ETH Press**, "Predictions of the effect of drugs on individual cells are now possible."	
2022	**MIT Press**, "Artificial intelligence system rapidly predicts how two proteins will attach."	
2014	**DKFZ News**, "Ring of Fire wins the world championship in synthetic biology."	
2014	**F.A.Z.**, "The Ring of Fire from Heidelberg."	

Professional Activities, Leadership, and Service

CONFERENCE AND WORKSHOP ORGANIZATION

2024 **Workshop Organizer**, Workshop on Learning Meaningful Representations of Life Singapore, SG
An ICLR workshop on learning representations of biology across scales and modalities using large-scale gen AI.

2024 **Workshop Organizer**, Workshop on Machine Learning for Genomics Explorations Vienna, Austria
An ICLR workshop bridging the gap between machine learning and genomics, with focus on target identification.

2023 **Workshop Organizer**, Workshop on Diffusion Models New Orleans, USA
A NeurIPS workshop on recent advances and future research directions of powerful diffusion generative models.

2023 **Workshop Organizer**, New Frontiers in Learning, Control, and Dynamical Systems Honolulu, USA
A new interdisciplinary ICML workshop discussing the interaction between control theory, and deep learning.

2022 **Founding Conference Organizer**, Molecular ML Conference (MoML) Cambridge, USA
Yearly conference on machine learning for molecular modeling, molecular interactions, and therapeutic design.

2021	**Workshop Organizer**, Optimal Transport and Machine Learning Workshop	New Orleans, USA

Bi-yearly NeurIPS workshop on recent advances and developments of optimal transport in machine learning.

2018	**Founding Conference Organizer**, Women in Data Science Conference (WiDS)	Zurich, Switzerland

Yearly technical conference featuring women's work in data science and adjacent engineering areas.

OPEN SOURCE CONTRIBUTIONS

- Python Library `OTT` for Optimal Transport Tools in JAX
- Python Library `PyCytominer` for Data Processing for Perturbation Profiling

PROFESSIONAL SERVICE

Editorial Board Member of the Machine Learning: Science and Technology (MLST) IOP Publishing journal.

Reviewer of Journals and Proceedings in Neural Information Processing Systems (NeurIPS), International Conference on Machine Learning (ICML), International Conference on Learning Representations (ICLR), International Conference on Artificial Intelligence and Statistics (AISTATS), Molecular Machine Learning (MoML) Conference, Nature Communications, and various workshops.

Publications

* authors contributed equally; + mentored student

Most recent publications via Google Scholar.

CONFERENCE AND JOURNAL PUBLICATIONS

Conference publications are archival and selectively refereed in Computer Science (acceptance rates ∼20 %).

Martin Rohbeck, **Charlotte Bunne**, Edward De Brouwer, Jan-Christian Huetter, Anne Biton, Kelvin Y. Chen, Aviv Regev, Romain Lopez. *Modeling Complex System Dynamics with Flow Matching Across Time and Conditions*. *International Conference on Learning Representations (ICLR)*, 2025.

Jayoung Ryu, Romain Lopez, **Charlotte Bunne**, Aviv Regev. *Cross-modality Matching and Prediction of Perturbation Responses with Labeled Gromov-Wasserstein Optimal Transport*. *International Conference on Artificial Intelligence and Statistics (AISTATS)*, 2025.
Best Paper Award and **Contributed Talk** at ICML AI for Science Workshop, 2024.

Erik Serrano, ..., **Charlotte Bunne**, ..., Anne E. Carpenter, Beth A. Cimini, Shantanu Singh, Gregory P. Way. *Reproducible image-based profiling with Pycytominer*. *Nature Methods*, 2025.

Charlotte Bunne, ..., Aviv Regev, Emma Lundberg, Jure Leskovec, Stephen R. Quake. *How to build the virtual cell with artificial intelligence: Priorities and opportunities*. *Cell*, 187:25 7045-7063, 2024.
Press Coverage in The Atlantic and **Guest in Ground Truths Podcast by Eric Topol**.

Charlotte Bunne, Geoffrey Schiebinger, Andreas Krause, Aviv Regev, Marco Cuturi. *Optimal transport for single-cell and spatial omics*. *Nature Reviews Methods Primer*, 2024.

Puck Gerwen, Ksenia Briling, **Charlotte Bunne**, Vignesh Ram Somnath, Ruben Laplaza, Andreas Krause, Clemence Corminboeuf. *3DReact: Geometric Deep Learning for Chemical Reactions*. *Journal of Chemical Information and Modeling*, 2023.

Charlotte Bunne*, Stefan Stark*, Gabriele Gut*, ..., Lucas Pelkmans, Andreas Krause, Gunnar Rätsch. *Learning Single-Cell Perturbation Responses using Neural Optimal Transport*. *Nature Methods*, 2023.
Selected as **Research Briefing** in Nature Methods.
Also presented at NeurIPS Workshop on Optimal Transport and Machine Learning, 2021.

Vignesh Ram Somnath*+, Matteo Pariset*+, Ya-Ping Hsieh, Maria Rodriguez Martinez, Andreas Krause, and **Charlotte Bunne**. *Aligned Diffusion Schrödinger Bridges*. *Uncertainty in Artificial Intelligence (UAI)*, 2023.

Charlotte Bunne*, Ya-Ping Hsieh*, Marco Cuturi, Andreas Krause. *The Schrödinger Bridge between Gaussian Measures has a Closed Form*. *International Conference on Artificial Intelligence and Statistics (AISTATS)*, 2023.
Oral Presentation at AISTATS (**Top 1.9 %** of Submitted Papers).
Presented at ICML Workshop on Continuous Time Methods for Machine Learning, 2022.

Charlotte Bunne, Andreas Krause, Marco Cuturi. *Supervised Training of Conditional Monge Maps*. *Advances in Neural Information Processing Systems (NeurIPS)*, 2022.
Also presented at ICML Workshop on Interpretable Machine Learning in Healthcare (IMLH), 2022.

Philippe Schwaller, Alain C. Vaucher, Ruben Laplaza, **Charlotte Bunne**, Andreas Krause, Clemence Corminboeuf, and Teodoro Laino. *Machine Intelligence for Chemical Reaction Space*. WIREs Computational Molecular Science, 2022.
Selected for **Featured Cover** of Volume 12, Issue 5

Charlotte Bunne, Laetitia Meng-Papaxanthos, Andreas Krause, and Marco Cuturi. *Proximal Optimal Transport for Population Dynamics. International Conference on Artificial Intelligence and Statistics (AISTATS)*, 2022.
Best Paper Award and **Contributed Talk** at ICML Time Series Workshop, 2021.

Octavian-Eugen Ganea*, Xinyuan Huang*[+], **Charlotte Bunne**, ..., and Andreas Krause. *Independent SE(3)-Equivariant Models for End-to-End Rigid Protein Docking. International Conference on Learning Representations (ICLR)*, 2021.
Spotlight Talk at ICLR and Ranked and Top 15 among 3326 Submissions (**Top 0.4 %**).
Also **Contributed Talk** at ELLIS Machine Learning for Molecule Discovery Workshop, 2021.

Charlotte Bunne*, Vignesh Ram Somnath*, and Andreas Krause. *Multi-Scale Representation Learning on Proteins. Advances in Neural Information Processing Systems (NeurIPS)*, 2021.
Also presented at ICML Computational Biology Workshop, 2021.

Vignesh Ram Somnath[+], **Charlotte Bunne**, Connor W. Coley, Andreas Krause, and Regina Barzilay. *Learning Template-Free Models for Retrosynthesis. Advances in Neural Information Processing Systems (NeurIPS)*, 2021.
Best Paper Award and **Contributed Talk** at ICML Workshop on Graph Representation Learning and Beyond

Matteo Manica*, **Charlotte Bunne***, Roland Mathis*, ..., María Rodríguez Martínez. *COSIFER: A Python Package for the Consensus Inference of Molecular Interaction Networks. Bioinformatics*, 2020.

Charlotte Bunne, David Alvarez-Melis, Andreas Krause, and Stefanie Jegelka. *Learning Generative Models across Incomparable Spaces. International Conference on Machine Learning (ICML)*, 2019.
Best Paper Award and **Contributed Talk** at NeurIPS Workshop on Relational Representation Learning, 2018.

Max Waldhauer, Silvan N. Schmitz, ..., **Charlotte Bunne**, ..., Roland Eils. *Backbone circularization of Bacillus subtilis family 11 xylanase increases its thermostability and its resistance against aggregation. Molecular BioSystems*, 2015.

Preprints and Under Submission

Johann Wenckstern*, Eeshaan Jain*, Kiril Vasilev, Matteo Pariset, Andreas Wicki, Gabriele Gut, **Charlotte Bunne**. *AI-powered virtual tissues from spatial proteomics for clinical diagnostics and biomedical discovery. Under Review at Cell (arXiv:2501.06039)*, 2025.

Matteo Pariset[+], Ya-Ping Hsieh, **Charlotte Bunne**, Andreas Krause, Valentin De Bortoli. *Unbalanced Diffusion Schrödinger Bridges. Preprint (arXiv:2306.09099)*, 2023.

Charlotte Bunne*, Frederike Lübeck*[+], Gabriele Gut, Jacobo Sarabia del Castillo, Lucas Pelkmans, David Alvarez-Melis. *Neural Unbalanced Optimal Transport via Cycle-Consistent Semi-Couplings. Preprint (arXiv:2209.15621)*, 2023.
Spotlight Presentation at NeurIPS Workshop on Learning Meaningful Representations of Life, 2022.

Marco Cuturi, Laetitia Meng-Papaxanthos, Yingtao Tian, **Charlotte Bunne**, Geoff Davis, Olivier Teboul. *Optimal Transport Tools (OTT): A JAX Toolbox for All Things Wasserstein. In Submission (arXiv:2201.12324)*, 2022.

Mathieu Chevalley[+], **Charlotte Bunne**, Andreas Krause, Stefan Bauer. *Invariant Causal Mechanisms through Distribution Matching. Preprint (arXiv:2206.11646)*, 2022.

Lisa Buchauer, Muhammad Amir Khan, ..., **Charlotte Bunne**, ..., Thomas Höfer, Hai-Kun Liu. *Exponential Growth of Glioblastoma In Vivo Driven by Rapidly Dividing and Outwardly Migrating Cancer Stem Cells. Preprint*, 2019.

Presentations

Talk Series

06/2024	**Lecture,** Personalized Medicine through Generative Modeling	Montreal, Canada
	ML for Drug Discovery Summer School of Recursion and Valence Labs	
07/2023	**Conference Tutorial,** Optimal Transport in Learning, Control, and Dynamical Systems	Honolulu, USA
	Tutorial at the International Conference on Machine Learning (ICML)	
11/2022	**Invited Talk,** Neural Optimal Transport for Inferring Single-Cell Perturbation Responses	Cambridge, USA
	Models, Inference & Algorithms (MIA) Initiative at the Broad Institute	
06/2022	**Invited Talk,** Optimal Transport Modeling of Single-Cell Dynamics	virtual
	Molecular Modeling And Drug Discovery Talks Series of Valence Discovery and Mila - Quebec AI Institute	
06/2020	**Invited Talk,** Learning across Incomparable Spaces (in Biomedical Applications)	virtual
	Data Science Seminar at the German Cancer Research Center	

Conference and Workshop Talks

06/2024	**Invited Talk,** Predicting Patient Treatment Outcomes using Generative Models CVPR Workshop on Computer Vision for Microscopy Image Analysis (CVMI)	Seattle, USA
04/2024	**Invited Talk,** Predicting Patient Treatment Outcomes using Generative Models AMLD Workshop on AI in Genomics	Lausanne, CH
11/2023	**Invited Talk,** Machine Learning-Guided Treatment Outcome Prediction and Planning Artificial Intelligence meets Cancer Research Symposium	Barcelona, Spain
09/2023	**Invited Talk,** Neural Optimal Transport for Treatment Outcome Prediction Conference on Generative Models and Uncertainty Quantification	Copenhagen, DK
07/2023	**Invited Talk,** Neural Optimal Transport for Single-Cell Biology Human Cell Atlas General Meeting	Toronto, Canada
06/2023	**Invited Talk,** Neural Optimal Transport for Inferring Single-Cell Perturbation Responses Workshop on Emerging Topics in Applications of Optimal Transport	Zurich, Switzerland
04/2023	**Invited Talk,** Optimal Transport Modeling of Population Dynamics Workshop on Optimal Transport, Mean-Field Models, and Machine Learning at TUM-IAS	Munich, Germany
09/2022	**Invited Talk,** Optimal Transport Modeling of Population Dynamics SIAM Conference on Mathematics of Data Science	San Diego, USA
03/2022	**Invited Talk,** Optimal Transport Modeling of Single-Cell Dynamics AMLD Conference Track 'AI in the Molecular World'	Lausanne, CH
07/2021	**Contributed Talk,** Proximal Optimal Transport Modeling of Population Dynamics ICML Time-Series Workshop	virtual
07/2021	**Contributed Talk,** Multi-Scale Representation Learning on Proteins ICML Computational Biology Workshop	virtual
12/2018	**Contributed Talk,** Learning Generative Models across Incomparable Spaces NeurIPS Workshop on Relational Representation Learning (R2L)	Montreal, Canada

Seminars at Universities

01/2023	**Invited Talk,** Neural Optimal Transport for Inferring Single-Cell Perturbation Responses Seminar at the German Cancer Research Center	Heidelberg, Germany
12/2022	**Invited Talk,** Neural Optimal Transport for Inferring Single-Cell Perturbation Responses Machine Learning Seminar at Stanford University	Palo Alto, USA
12/2022	**Invited Talk,** Neural Optimal Transport for Inferring Single-Cell Perturbation Responses Machine Learning Seminar at Dana-Farber Cancer Institute	Boston, USA
09/2022	**Invited Talk,** Modeling (Combination) Therapy Outcomes using Optimal Transport Computational Health Center at Helmholtz Munich	Munich, Germany
08/2022	**Invited Talk,** Optimal Transport Modeling of Single-Cell Dynamics Imaging Platform of the Broad Institute	Cambridge, USA
06/2022	**Invited Talk,** Optimal Transport Modeling of Population Dynamics StatEcoML Seminar of ENSAE - CREST	Paris, France
06/2022	**Invited Talk,** Dynamic Models for Cell Dynamics and Protein Modeling AI for Science Group at Humboldt University of Berlin	Berlin, Germany
06/2022	**Invited Talk,** Optimal Transport Modeling of Population Dynamics in Single-Cell Biology Berlin Institute of Health (BIH)	Berlin, Germany

Seminars at Industry Research Labs

06/2024	**Invited Talk,** Predicting Patient Treatment Outcomes using Generative Models NVIDIA	Santa Clara, USA
12/2022	**Invited Talk,** Neural Optimal Transport for Inferring Single-Cell Perturbation Responses Genentech	San Francisco, USA
12/2022	**Invited Talk,** Neural Optimal Transport for Population Dynamics Apple	Cupertino, USA
11/2022	**Invited Talk,** Modeling (Combination) Therapy Outcomes using Optimal Transport Microsoft Research	Cambridge, USA
03/2022	**Invited Talk,** Optimal Transport Modeling of Population Dynamics MIT-IBM Watson AI Lab	virtual

09/2021	**Invited Talk,** Proximal Optimal Transport Modeling of Population Dynamics	virtual
	Diff-Everything Workshop at Google Research	
11/2019	**Invited Talk,** Learning Generative Models across Incomparable Spaces	Zurich, Switzerland
	IBM Research	

Teaching

UNIVERSITY COURSES AT ETH ZURICH

All taught classes consist of lectures, tutorials, and practical projects.

Spring 2023	**Teaching Assistant,** Introduction to Machine Learning	*Zurich, Switzerland*
Fall 2022	**Teaching Assistant,** Probabilistic Artificial Intelligence	
Fall 2021	**Head Teaching Assistant,** Introduction to Machine Learning	
Spring 2021	**Head Teaching Assistant,** Introduction to Machine Learning ($\sim$1000 Students)	
Fall 2020	**Teaching Assistant,** Probabilistic Artificial Intelligence	
Spring 2020	**Teaching Assistant,** Introduction to Machine Learning	
Fall 2019	**Teaching Assistant,** Probabilistic Artificial Intelligence	
Spring 2019	**Teaching Assistant,** Fairness, Explainability, & Accountability for Machine Learning	

Supervision

since 2024	**Johann Wenckstern,** PhD Student, EPFL
	EPFL EDIC Fellowship.
since 2024	**Eeshaan Jain,** PhD Student, EPFL
	EPFL EDIC Fellowship.
2023-2024	**Johann Wenckstern,** Master Student, ETH Zurich
	Co-supervision with the Unispital Zürich.
2023	**Alexander Hägele,** Master Student, ETH Zurich and Apple
	Co-supervision with Marco Cuturi (Apple) and Andreas Krause (ETH Zurich).
2023	**Yunshu Ouyang,** Master Student, Broad Institute of MIT and Harvard
	Co-supervision with Jiaqi Zhang and Caroline Uhler (MIT).
2022-2023	**Matteo Pariset,** Master Student, EPFL
	Resulting paper accepted at UAI 2023 and awarded best thesis prize at EPFL.
2022-2023	**Frederike Lübeck,** Master Student, Harvard University
	Co-supervision with David Alvarez Melis (Harvard). Resulting paper got spotlight at NeurIPS workshop.
2020-2021	**Mathieu Chevalley,** Master Student,
	Co-supervision with Stefan Bauer (TUM).
2020-2021	**Xinyuan Huang,** Master Student, ETH Zurich
	Co-supervision with Octavian Ganea (MIT). Resulting paper got a spotlight presentation (top 0.4%) at ICLR 2022.
2019-2020	**Kenza Amara,** Master Student, ETH Zurich
	Co-supervision with David Dao (ETH).
2019-2020	**Vignesh Ram Somnath,** Master Student, Massachusetts Institute of Technology (MIT)
	Co-supervision with Regina Barzilay. Resulting publication received *Best Paper Award* at ICML Workshop 2020.

Languages and Skills

Computer Skills
Languages: *Python, MATLAB, R, Git, SQL, LaTeX*
Libraries: *JAX, PyTorch, TensorFlow, SciKit*

Languages
German and English: Native and Fluent
French: Conversant