

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 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

2025	Best Paper Award , ICLR Machine Learning for Genomics Explorations Workshop	1/55 Papers
2024	ETH Medal , ETH Zurich	Best PhD Thesis, Top 2.5%
2024	Best Paper Award , ICML AI for Science Workshop	1/148 Papers

2024	SIB Remarkable Outputs 2023 Award , SIB Swiss Institute of Bioinformatics	
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	Best Master Thesis, Top 2.5%
	Willi Studer Prize , ETH Zurich	Best GPA in Study Program
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

2025	AI2050 Early Career Award , Schmidt Sciences	
	\$ 0.5M for the 'Biological World Models for AI-Driven Reasoning and Decision Support'.	
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 <i>most prestigious</i> 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

2025	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

Kiril Vasilev*, Alexandre Misrahi*, Eeshaan Jain*, Phil Cheng, Petros Liakopoulos, Olivier Michielin, Michael Moor, **Charlotte Bunne**. *CRONOS: A Multimodal Sequential Clinical Decision-Making Benchmark in Oncology*. *Under Review at NeurIPS Datasets and Benchmark Track*, 2025.

Eeshaan Jain, Johann Wenckstern, Benedikt von Querfurth, **Charlotte Bunne**. *Test-Time View Selection for Multi-Modal Decision Making*. *Under Review at Cell*, 2025.
Contributed Talk at ICLR MLGenX Workshop, 2025.

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 (arXiv:2501.06039)*, 2025.
Best Paper Award at ICLR MLGenX Workshop, 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.

Invited Talks, Panels, Lectures, and Keynotes

12/2025	Colloquium , Eric and Wendy Schmidt Center at the Broad Institute	Cambridge, USA
07/2025	Invited Talk , AACR Special Conference in Cancer Research on Artificial Intelligence	Montreal, Canada
06/2025	Invited Talk , Foundation Models in Cellular Biology (AI x Bio) Conference	Cambridge, UK

05/2025	Invited Talk , CIFAR MacMillan Multiscale Human Program Meeting	Geneva, CH
04/2025	Keynote , ICLR Workshop on Machine Learning Multiscale Processes	Singapore, SG
04/2025	Panel Discussion and Keynote , ICLR GemBio Workshop	Singapore, SG
04/2025	Keynote , ICLR Workshop on Artificial Intelligence for Nucleic Acids	Singapore, SG
03/2025	Invited Talk , AI in Drug Discovery and Biomedicine	Barcelona, Spain
02/2025	Keynote , AMLD Workshop on AI in Comp. Biology: From Molecules to Medicine	Lausanne, CH
02/2025	Invited Talk , AGORA Internal Seminar	Lausanne, CH
01/2025	Keynote , Statistical Methods for Post Genomic Data	Heidelberg, Germany
01/2025	Invited Talk , Physics of AI Algorithms (PHAIA)	Les Houches, France
01/2025	Invited Talk , heidelberg.ai	Heidelberg, Germany
12/2024	Invited Talk , CECAM Workshop on Combining AI and Physical Modeling	Lausanne, CH
09/2024	Invited Talk , Workshop on Spatial and Temporal Statistical Modeling in Biology	Ascona, CH
07/2024	Keynote , ICML Workshop on Structured Probabilistic Inference & Generative Modeling	Vienna, Austria
06/2024	Lecture , ML for Drug Discovery Summer School of Recursion and Valence Labs	Montreal, Canada
06/2024	Lecture , ML for Drug Discovery Summer School of Recursion and Valence Labs	Montreal, Canada
06/2024	Invited Talk , CVPR Workshop on Computer Vision for Microscopy Image Analysis	Seattle, USA
06/2024	Invited Talk , NVIDIA	Santa Clara, USA
04/2024	Invited Talk , AMLD Workshop on AI in Genomics	Lausanne, CH
07/2023	Conference Tutorial , OT in Learning, Control, and Dynamical Systems at ICML	Honolulu, USA
07/2023	Invited Talk , Human Cell Atlas General Meeting	Toronto, Canada
11/2023	Invited Talk , Artificial Intelligence meets Cancer Research Symposium	Barcelona, Spain
09/2023	Invited Talk , Conference on Generative Models and Uncertainty Quantification	Copenhagen, DK
06/2023	Invited Talk , Workshop on Emerging Topics in Applications of Optimal Transport	Zurich, CH
04/2023	Invited Talk , Workshop on Optimal Transport, Mean-Field Models, and ML at TUM-IAS	Munich, Germany
01/2023	Invited Talk , Seminar at the German Cancer Research Center	Heidelberg, Germany
12/2022	Invited Talk , Machine Learning Seminar at Stanford University	Palo Alto, USA
12/2022	Invited Talk , Machine Learning Seminar at Dana-Farber Cancer Institute	Boston, USA
12/2022	Invited Talk , Genentech	San Francisco, USA
12/2022	Invited Talk , Apple	Cupertino, USA
11/2022	Invited Talk , Models, Inference & Algorithms (MIA) Initiative at the Broad Institute	Cambridge, USA
11/2022	Invited Talk , Microsoft Research	Cambridge, USA
06/2022	Invited Talk , Molecular Modeling And Drug Discovery (M2D2) at Valence Labs	Virtual
06/2022	Invited Talk , StatEcoML Seminar of ENSAE - CREST	Paris, France
06/2022	Invited Talk , AI for Science Group at Humboldt University of Berlin	Berlin, Germany
03/2022	Invited Talk , AMLD Conference Track 'AI in the Molecular World'	Lausanne, CH
03/2022	Invited Talk , MIT-IBM Watson AI Lab	Virtual
07/2021	Contributed Talk , ICML Time-Series Workshop	Virtual
07/2021	Contributed Talk , ICML Computational Biology Workshop	Virtual
06/2020	Invited Talk , Data Science Seminar at the German Cancer Research Center	Virtual
12/2018	Contributed Talk , NeurIPS Workshop on Relational Representation Learning (R2L)	Montreal, Canada

Teaching

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

UNIVERSITY COURSES AT EPFL

Fall 2025 **Lecturer**, Foundation Models and Generative Artificial Intelligence *Lausanne, CH*

UNIVERSITY COURSES AT ETH ZURICH

2020 - 2023 **Teaching Assistant**, Introduction to Machine Learning *Zurich, CH*
2019 - 2022 **Teaching Assistant**, Probabilistic Artificial Intelligence
2019 **Teaching Assistant**, Fairness, Explainability, & Accountability for Machine Learning

Supervision

- since 2025 **Linus Bleistein**, PostDoctoral Fellow, EPFL
EPFL AI Center PostDoctoral Fellow.
- since 2025 **Lukas Klein**, PostDoctoral Fellow, EPFL and USZ
Co-supervised by Andreas Wicki (USZ).
- 2025 **Alexandre Misrahi**, Master Student, EPFL
- 2025 **Kiril Vasilev**, Master Student, EPFL
Co-supervised by Michael Moor (ETH Zurich).
- 2025 **Maria Vittoria Impagliazzo**, Master Student, EPFL
Co-supervised by Bart Deplancke (EPFL).
- since 2024 **Johann Wenckstern**, PhD Student, EPFL
EPFL EDIC Fellowship.
- since 2024 **Eeshaan Jain**, PhD Student, EPFL
EPFL EDIC Fellowship.
- since 2024 **Benedikt von Querfurth**, Research Scholar, EPFL
- since 2024 **Yexiang Chen**, Research Scholar, EPFL
- 2023-2024 **Johann Wenckstern**, Master Student, ETH Zurich
Co-supervised by Andreas Wicki (USZ).
- 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 Zurich).
- 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, $\text{\LaTeX}$*
Libraries: *JAX, PyTorch, TensorFlow, SciKit*

Languages

German and English: Native and Fluent
French: Conversant