

# Luis Müller

Aachen, Germany

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## Education

- 2022 – Present **RWTH Aachen University** – Aachen, Germany  
*PhD student*, developing a principled understanding of how transformers can be applied to graph learning.  
Advisor: Christopher Morris
- 2019 – 2022 **TU Berlin** – Berlin, Germany  
*M.Sc. Computer Science* with a focus on Machine Learning and Robotics.  
Graduated with the highest possible grade (1.0).
- 2015 – 2020 **TU Berlin** – Berlin, Germany  
*B.Sc. Computer Science*

## Selected Works

- NeurIPS 2024 **Towards Principled Graph Transformers**  
**Luis Müller**, Daniel Kusuma, Blai Bonet, Christopher Morris
- ICML 2024 **Aligning Transformers with Weisfeiler–Leman**  
**Luis Müller**, Christopher Morris
- AccMLBio workshop at ICML 2024 **MiniMol: A Parameter-Efficient Foundation Model for Molecular Learning**  
Kerstin Kläser, Błażej Banaszcwski, Samuel Maddrell-Mander, Callum McLean, **Luis Müller**, Ali Parviz, Shenyang Huang, Andrew Fitzgibbon
- ICLR 2024 **Towards Foundational Models for Molecular Learning on Large-Scale Multi-Task Datasets**  
Dominique Beaini, Shenyang Huang, Joao Alex Cunha, Zhiyi Li, Gabriela Moisescu-Pareja, Oleksandr Dymov, Samuel Maddrell-Mander, Callum McLean, Frederik Wenkel, **Luis Müller**, Jama Hussein Mohamud, Ali Parviz, Michael Craig, Michał Koziarski, Jiarui Lu, Zhaocheng Zhu, Cristian Gabellini, Kerstin Kläser, Josef Dean, Cas Wognum, Maciej Sypetkowski, Guillaume Rabusseau, Reihaneh Rabbany, Jian Tang, Christopher Morris, Ioannis Koutis, Mirco Ravanelli, Guy Wolf, Prudencio Tossou, Hadrien Mary, Therence Bois, Andrew Fitzgibbon, Błażej Banaszcwski, Chad Martin, Dominic Masters
- TMLR **Attending to Graph Transformers**  
**Luis Müller**, Mikhail Galkin, Christopher Morris, Ladislav Rampásek

ADT 2021     **On Reachable Assignments in Cycles** (work done as undergrad)  
Luis Müller, Matthias Bentert

## Academic Experience

Reviewing	NeurIPS 2024, ICLR 2025 and TMLR.
Teaching	Supervision of Bachelor's and Master's thesis students as well as student assistants. Held two lectures (1.5h each) on Transformers for Graphs for Master's students at RWTH Aachen University in summer 2024.
Community	Co-organizer of the Graph Learning on Wednesdays reading group and co-organizer of the Learning on Graphs Conference ( <a href="https://logconference.org">https://logconference.org</a> ).
Talks	Talks about my scientific work, at the Transformer reading group at Mila ( <a href="https://www.youtube.com/watch?v=BuNXQIzLBWc">https://www.youtube.com/watch?v=BuNXQIzLBWc</a> ), and at Haggai Marons' lab ( <a href="https://haggaim.github.io">https://haggaim.github.io</a> ).
Software	Contributor to GraphGPS ( <a href="https://github.com/rampasek/GraphGPS">https://github.com/rampasek/GraphGPS</a> ) and core-contributor to Graphium ( <a href="https://github.com/datamol-io/graphium">https://github.com/datamol-io/graphium</a> ).
Summer Schools	Machine Learning Summer School (MLSS) 2024, EEML summer school 2022 (awarded with a best poster award).

## Industry experience

2021 – 2022	<b>NVT Sustainability Engagement Team at SAP (Working Student)</b> – Berlin, Germany Design, innovation and product development in the area of sustainability, including machine learning applications.
2017 – 2021	<b>Promos Consult (Working Student)</b> – Berlin, Germany Full-stack software development.

## Technical skills

Programming	Python, Java, JavaScript, C/C++, Julia.
ML software	PyTorch, Jax, TensorFlow, NumPy, Pandas, PyBind11 (C/C++ bindings into Python).
Software development	Git/Github, experience with writing and testing production-ready code, including code review and developing in large codebases.
Languages	English (fluent), German (native speaker), Norwegian (intermediate).