

Magdalena Lederbauer

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EDUCATION

Massachusetts Institute of Technology 2025-present
PhD Chemical Engineering and Computing (CSE-ChemE) Cambridge, MA, USA
Entalpic Research Fellow

ETH Zurich 2023–2025
MSc Chemistry, graduated with distinction Zurich, Switzerland
Selected into the **Excellence Scholarship & Opportunity Program** awarded to top 2% students
Master's thesis awarded with **ETH medal** (top 2.5% of all graduates), **S&N Blank Prize** for best thesis in organic and polymer chemistry. Graduated top of class (**Willi Studer Prize**).

ETH Zurich 2020–2023
BSc Chemistry, graduated with distinction Zurich, Switzerland
Received **Excellence Scholarship** for studies abroad, awarded to three students in Lower Austria
Selected as Fellow of the **Swiss Academic Study Foundation** (Schweizerische Studienstiftung) and the **Austrian Academic Study Foundation** (Österreichische Studienstiftung)

RESEARCH & WORK EXPERIENCE

MIT, Chemical Engineering 01/26–present
Graduate Student Cambridge, MA, USA
Supervisors: Prof. Dr. **Connor W. Coley**
Research focus on developing machine learning methods for molecular structure elucidation from mass spectrometry data and reaction discovery, with an emphasis on physics-constrained neural networks and generative models.

Entalpic 05/25–08/25
Visiting Machine Learning Scientist in Chemistry Paris, France
Data curation and large language models (LLMs) for the automated discovery of catalysts to decarbonize industrial chemistry. Lead of an internal project of six scientists and engineers, lead of an open source project (*LeMaterial, vide infra*) of 20 members.

MIT, Chemical Engineering 10/24–03/25
Visiting Graduate Student Cambridge, MA, USA
Supervisors: Prof. Dr. **Connor W. Coley**, Dr. Runzhong Wang
Structure elucidation from mass spectrometry using neural networks. Developed pipeline for analyzing pesticides and biomarkers with LC-MS/MS and GC-EI/MS data.

EPFL, Laboratory of Artificial Chemical Intelligence 03/24–07/24
Intern Lausanne, Switzerland
Supervisors: Prof. Dr. **Philippe Schwaller**, Andrès M. Bran
LLM Agents in Heterogeneous Single Atom Catalysis. Built an LLM pipeline and graphical user interface to curate and predict synthesis procedures.

ETH Zurich, Energy Systems Process Engineering Group 04/22–06/23
Research Assistant Zurich, Switzerland
Group of Prof. Dr. **André Bardow**, Dr. Benedikt Winter
Predicting Molecular Properties and Binary Phase Diagrams with a SMILES-to-Property-Transformer.

SELECTED AWARDS

Fellowships, Grants and Scholarships

- Entalpic Research Fellowship** 2026
Selective fellowship supporting PhD research in AI for materials science with financial support and scientific mentorship. One of three awardees.
- Lindau Spirit Fellowship** 2025
Fellowship to participate in the 74th Lindau Nobel Laureate Meetings in Chemistry, one of seven awardees. Additional travel grant awarded by the Austrian Study Foundation (Austrian Academy of Sciences).
- Zeno Karl Schindler Foundation Master Thesis Grant** 2024
Merit-based excellence scholarship for master's theses in engineering disciplines. Top 10%.
- Swiss-European Mobility Programme (SEMP) Scholarship** 2024
ETH Zurich. Scholarship for exchange abroad.
- Travel Grant by the Study Foundation ("Zuschuss")** 2024
Swiss Study Foundation. Travel grant for conference visit in Oxford, UK.
- Excellence Scholarship and Opportunity Programme (ESOP)** 2023
ETH Zurich. Merit-based excellence scholarship for master's studies at ETH Zurich. Top 2%.
- Exzellenzstipendium Ausland - Excellence Scholarship for studies abroad** 2020
Lower Austrian Society for Research Promotion. Merit-based excellence scholarship for bachelor studies at ETH Zurich. One of three awardees.

Prizes

- ETH Medal** 2025
Awarded for outstanding master's thesis, awarded to top 2.5% of graduates of ETH Zurich.
- S&N Blank Prize** 2025
Awarded for the best master's thesis in organic and polymer chemistry at ETH Zurich.
- Willi-Studer Prize** 2025
Awarded to the best master's degree graduate at ETH Zurich. Best overall GPA in Chemistry.
- Chemical Science Journal Poster Prize** 2024
Royal Society of Chemistry. Awarded to top poster presentation at Faraday Discussions, Oxford, UK.
- Physical Chemistry Chemical Physics Journal Poster Prize** 2024
Royal Society of Chemistry. Awarded to top poster presentation at Chemical Compound Space Conference (CCSC), Heidelberg, Germany.
- Dr. Hans Riegel Fachpreis (1st place in Chemistry)** 2020
University of Vienna / Kaiserschild Foundation. Awarded to top high school research projects in chemistry in Germany and Austria.
- Institute of Science and Technology Austria (ISTA) school award** 2020
Institute of Science and Technology Austria (ISTA). Awarded to top high school research projects in STEM in Austria.
- Agnes-Ruis-Prize for best experimental chemistry project** 2020
Society of Austrian Chemists (GÖCH). Awarded to best experimental research high school project in chemistry in Austria.

Competitions

- Lila Sciences Prize and MIT on-site Prize** 2025
Worldwide LLM Hackathon for Applications in Materials Science and Chemistry. Top 3/120 submissions (top 3%).

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| Second place & Knowledge Graph Prize | 2024 |
| <i>Worldwide LLM Hackathon for Applications in Materials Science and Chemistry. Top 2/34 submissions (top 6%).</i> | |
| Impact Potential Prize | 2023 |
| <i>Swiss Data Science Center (SDSC) Generative AI Hackathon</i> | |
| Silver Medals | 2019, 2020 |
| <i>52nd and 51st International Chemistry Olympiads</i> | |
| First place | 2019, 2020 |
| <i>45th and 46th Austrian National Chemistry Olympiads</i> | |
| Silver Medal | 2019 |
| <i>53rd International Mendeleev Chemistry Olympiad</i> | |
| First place | 2019 |
| <i>Students' competition of the University of Vienna. Topic "How Can We Save Our Climate?"</i> | |
| Second place and audience award | 2018 |
| <i>Students' competition of the University of Vienna. Topic "Health Out Of The Lab"</i> | |
| Bronze Medal | 2018 |
| <i>50th International Chemistry Olympiad</i> | |
| Silver Medal | 2018 |
| <i>European Science Olympiad (EUSO, now EOES). Interdisciplinary team competition in physics, biology and chemistry. Chemist of Team Austria A.</i> | |

SELECTED PRESENTATIONS

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| Invited Tutorial | 08/2025 |
| <i>LLM Hackathon for Applications in Materials and Chemistry</i> | |
| | online |
| Invited Talk | 06/2025 |
| <i>74th Lindau Nobel Laureate Meetings in Chemistry</i> | |
| | Lindau, Germany |
| "Structure Elucidation of Unknown Molecules With Physics-Constrained Neural Simulators of Electron Ionization Mass Spectrometry". Nine speakers chosen among cohort of 600+ young scientists. | |
| Invited Talk | 2024 |
| <i>Annual ETH Zurich Foundation donor event</i> | |
| | Zurich, Switzerland |

SELECTED PUBLICATIONS

1. **M. Lederbauer**, S. Betala, X. Li, A. Jain, A. Sehaba, G. Channing, G. Germain, A. Leonescu, F. Flaifil, A. Amayuelas, A. Nozadze, S. Schmid, M. Zaki, S. Kumar Ethirajan, E. Pan, M. Franckel, A. Duval, N M A. Krishnan, S. Gleason, LeMat-Synth: a multi-modal toolbox to curate broad synthesis procedure databases from scientific literature. arXiv:2510.26824 (2025).
2. R. Wang, M. Manjrekar, B. Mahjour, J. Avila-Pacheco, J. Provenzano, E. Reynolds, **M. Lederbauer**, E. Mashin, S. L. Goldman, M. Wang, J.-K. Weng, D. L. Plata, C. B. Clish, C. W. Coley, Neural Spectral Prediction for Structure Elucidation with Tandem Mass Spectrometry. *bioRxiv* (2025).
3. **M. Lederbauer**, Learning Chemical Intuition: From Molecular Models to Neural Networks: Chemical Education. *CHIMIA* **79**, 174175 (2025).
4. G. P. Wellawatte, H. Guo, **M. Lederbauer**, A. Borisova, M. Hart, M. Brucka, P. Schwaller, ChemLit-QA: a human evaluated dataset for chemistry RAG tasks. *Mach. Learn.: Sci. Technol.* **6**, 020601 (2025).

TEACHING

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| Head Teaching Assistant | 2023 |
| <i>Inorganic Chemistry I (Coordination Chemistry and Spectroscopy), led team of five TAs and 180+ undergraduate students</i> | |
| Teaching Assistant | 2022 |
| <i>Inorganic Chemistry I (Coordination Chemistry and Spectroscopy)</i> | |
| Teaching Assistant | 2022 |
| <i>Physical Chemistry I (Thermodynamics)</i> | |
| Teaching Assistant | 2021 |
| <i>General Inorganic Chemistry I</i> | |
| Tutor | 2021, 2024 |
| <i>Austrian Chemistry Olympiad, Tutor in Organic Chemistry</i> | |
| Trainer | 2018-21 |
| <i>European Science Olympiad, Trainer in Chemistry</i> | |

PROFESSIONAL ACTIVITIES, LEADERSHIP, AND SERVICE

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| Communication Fellow @ MIT Chemical Engineering | 2026-present |
| <i>Offers support in writing, speaking, and visual design support for undergraduate students, graduate students, and post-docs in Engineering.</i> | |
| MoML @ MIT | 2026-present |
| <i>Co-organizer of the conference Molecular Machine Learning at MIT, Cambridge, USA.</i> | |
| Simulators @ ICML | 2026-present |
| <i>Co-organizer of the workshop "Simulations to Science" at ICML 2026 in Seoul, Korea.</i> | |
| Young Swiss Chemical Society (youngSCS) | 2021-24 |
| <i>ETH Representative, Board Member and International Relations representative</i> | |
| International Olympiads (IChO, EUSO) | 2018-23 |
| <i>Exam Co-Author for the 55th IChO 2023 in Switzerland: drafted, created and corrected 340+ exams. Tutor (2018-19) for the European Science Olympiad (EUSO, now EOES) Co-lead in chemistry for the training days for the national selection round and final training days for Team Austria and Team Germany.</i> | |
| Women in Natural Sciences at ETH Zurich (WiNS) | 2021-24 |
| <i>Association representing all female researchers in Chemistry, Chemical Engineering, Biology, Physics and Material Science at ETH Zurich. First-ever Student Representative (2021-22) and Webmaster (2022-24): building website and backend from the bottom-up.</i> | |

OPEN SOURCE

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| LeMaterial | 2025-present |
| <i>Lead of the working group "Large Language Models for Materials Synthesis Extraction", coordination of collaboration with 20+ participants. Leading effort for developing the database and manuscript.</i> | |
| Open Textbook for computational mass spectrometry | 2026-present |
| <i>Collaboration within the European Bioinformatics Society for Mass Spectrometry (EuBIC). Contributor to the section "machine learning for structure elucidation from mass spectrometry".</i> | |

MISCELLANEOUS

Languages: German (Native), English (Fluent), French (Conversant)
Reviewing: NeurIPS AI for Accelerated Materials Discovery (AI4Mat) 2025 (**Outstanding Reviewer**), ICLR AI4Mat 2026