



# Magdalena Lederbauer

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## EDUCATION

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

**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 at MIT (Group of Prof. Dr. Connor W. Coley)

**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

**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 decarboxylate 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**, Andr s 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, Digital Chemistry Laboratory** 09/23–12/23  
*Research Project* Zurich, Switzerland  
Supervisors: Prof. Dr. **Kjell J rner**, Vignesh Ram Somnath (with Prof. Dr. **Andreas Krause**)  
Multi-Scale Representations for Predicting Surface Reactivity of Molecules with GNNs.

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

**ETH Zurich, Cop ret Group** 02/23–05/23  
*Research Project* Zurich, Switzerland  
Supervisors: Prof. Dr. **Christophe Cop ret**, Dr. Zachariah Berkson  
Decoding Solid-State NMR Descriptors using Machine Learning with a large *in silico* DFT dataset.

## SELECTED AWARDS

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### Fellowships, Grants and Scholarships

<b>Lindau Spirit Fellowship</b>	2025
<i>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).</i>	
<b>Zeno Karl Schindler Foundation Master Thesis Grant</b>	2024
<i>Merit-based excellence scholarship for master's theses in engineering disciplines. Top 10%.</i>	
<b>Swiss-European Mobility Programme (SEMP) Scholarship</b>	2024
<i>ETH Zurich. Scholarship for exchange abroad.</i>	
<b>Travel Grant by the Study Foundation ("Zuschuss")</b>	2024
<i>Swiss Study Foundation. Travel grant for conference visit in Oxford, UK.</i>	
<b>Excellence Scholarship and Opportunity Programme (ESOP)</b>	2023
<i>ETH Zurich. Merit-based excellence scholarship for master's studies at ETH Zurich. Top 2%.</i>	
<b>Exzellenzstipendium Ausland - Excellence Scholarship for studies abroad</b>	2020
<i>Lower Austrian Society for Research Promotion. Merit-based excellence scholarship for bachelor studies at ETH Zurich. One of three awardees.</i>	

### Competitions

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

### Conferences and Research

<b>Chemical Science Journal Poster Prize</b>	2024
<i>Royal Society of Chemistry. Awarded to top poster presentation at Faraday Discussions, Oxford, UK.</i>	
<b>Physical Chemistry Chemical Physics Journal Poster Prize</b>	2024
<i>Royal Society of Chemistry. Awarded to top poster presentation at Chemical Compound Space Conference (CCSC), Heidelberg, Germany.</i>	

- European Forum Alpbach** 2020  
*Participation and scholarship to attend the Forum Alpbach, a global think-tank.*
- 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.*

## SELECTED PRESENTATIONS

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- Invited Tutorial** 08/2025  
*LLM Hackathon for Applications in Materials and Chemistry* online
- Invited Talk** 06/2025  
*74th Lindau Nobel Laureate Meetings in Chemistry* 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.
- Poster Presentation** 2024  
*Faraday Discussions on Data-driven discovery in the chemical sciences* Oxford, UK  
 "Toward A General Synthesis Planning Tool for Single Atom Catalysis". Awarded poster prize.
- Invited Talk** 2024  
*Annual ETH Zurich Foundation donor event* Zurich, Switzerland  
 "Digital Chemistry: A Paradigm Shift", speaker chosen among cohort of 200+ scholarship holders. Held in German.
- Poster Presentation** 2024  
*Chemical Compound Space Conference (CCSC) 2024* Heidelberg, Germany  
 "Decoding Solid-State NMR Descriptors Using Machine Learning: A Transition Metal Dataset". Awarded first poster prize (1st out of 60).
- Poster Presentation** 2023  
*Swiss Chemical Society Fall Meeting* Bern, Switzerland  
 "Decoding Solid-State NMR Descriptors Using Machine Learning".

## SELECTED PUBLICATIONS

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1. **M. Lederbauer**, Learning Chemical Intuition: From Molecular Models to Neural Networks: Chemical Education. *CHIMIA* **79**, 174175 (2025).
2. 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).

## Conference submissions

1. A. Oarga, M. Hart, A. M. Bran, **M. Lederbauer**, P. Schwaller, Scientific Knowledge Graph and Ontology Generation using Open Large Language Models. *NeurIPS 2024 Workshop FM4Science and NeurIPS 2024 Workshop AI4Mat* (2024). **Spotlight presentation (top 10-15%)**.
2. 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. *NeurIPS 2024 Workshop ML4PS*. **Spotlight presentation (top 10-15%)**.

## Preprints

1. 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).

## TEACHING

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

## OUTREACH

<b>Women in Natural Sciences at ETH Zurich (WiNS)</b>	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>	
<b>International Olympiads (IChO, EUSO)</b>	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>	

## OPEN SOURCE PROJECTS

<b>LeMaterial</b>	2025-present
<i>Lead of the working group "Large Language Models for Materials Synthesis Extraction" (LeMat-Synth), coordination of weekly project meetings with 20+ participants. Leading effort for developing the database and manuscript.</i>	

## MISCELLANEOUS

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

## PRESS

For an overview of press appearances, please refer to [here](#).