Magdalena Lederbauer

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EDUCATION

ETH Zurich   2023 – 2025 (expected)
MSc Chemistry   Zurich, Switzerland

- Focus Digital Chemistry, Catalysis Engineering, Spectroscopy
- Selected into the **Excellence Scholarship & Opportunity Program** (ESOP) awarded to top 2% students
- Master's thesis at **MIT** supported by the **Swiss European Mobility Programme** and merit-based **Zeno Karlo Schindler Master Thesis Grant**

ETH Zurich   2020 – 2023
BSc Chemistry   Zurich, Switzerland

- Graduated with distinction (average 5.82/6.00)
- Received the **Excellence Scholarship** for studies abroad, awarded to top 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 AND WORK EXPERIENCE

10/24-present	**MIT, Chemical Engineering**, *Visiting Graduate Student* Supervisors: Prof. Dr. **Connor W. Coley**, Dr. Runzhong Wang Structure elucidation from mass spectrometry using neural networks	*Cambridge, MA, USA*
03/24-07/24	**EPFL, Laboratory of Artificial Chemical Intelligence**, *Internship* Supervisors: Prof. Dr. **Philippe Schwaller**, Andrès M. Bran Large Language Model (LLM) Agents in Heterogeneous Single Atom Catalysis Built LLM pipeline to predict synthesis procedures Work presented at Faraday Discussions 2024, Oxford, UK (awarded best poster prize)	*Lausanne, Switzerland*
09/23-12/23	**ETH Zurich, Digital Chemistry Laboratory**, *Research Project* Supervisors: Prof. Dr. **Kjell Jorner**, Vignesh Ram Somnath (with Prof. Dr. **Andreas Krause**) Multi-Scale Representations for Predicting Surface Reactivity of Molecules with GNNs	*Zurich, Switzerland*
04/22-06/23	**ETH Zurich, Mechanical and Process Engineering**, *Research Project* Supervisors: Prof. Dr. **André Bardow**, Benedikt Winter Predicting Molecular Properties and Phase Diagrams with a SMILES-to-Property-Transformer Trained and evaluated models qualitatively and quantitatively Pipeline built into commercialized software (2% ownership)	*Zurich, Switzerland*
02/23-05/23	**ETH Zurich, Copéret Group**, *Research Project* Supervisors: Prof. Dr. **Christophe Copéret**, Dr. Zachariah Berkson Decoding Solid-State NMR Descriptors using Machine Learning Work presented at Chemical Compound Space Conference 2023, Heidelberg, Germany (awarded best poster prize)	*Zurich, Switzerland*

Selected Fellowships

2024   **Zeno Karl Schindler Foundation Master Thesis Grant**, *Merit-based excellence scholarship for master's theses in engineering disciplines. Top 10%.*

2024   **Swiss-European Mobility Programme (SEMP) Scholarship**, *ETH Zurich. Scholarship for exchange abroad.*

2023   **Excellence Scholarship and Opportunity Programme (ESOP)**, *ETH Zurich. Merit-based excellence scholarship for master's studies at ETH Zurich. Top 2%.*

2020   **Exzellenzstipendium Ausland - Excellence Scholarship**, *Lower Austrian Society for Research Promotion. Merit-based excellence scholarship for bachelor studies at ETH Zurich. One of three awardees.*

Competitions

2024   **2nd Place & Knowledge Graph Prize**, *Worldwide LLM Hackathon for Applications in Materials Science and Chemistry*

2023   **Impact Potential Prize**, *Swiss Data Science Center (SDSC) Generative AI Hackathon*

2020   **Silver Medal**, *52nd International Chemistry Olympiad*

2020   **1st place**, *Austrian National Chemistry Olympiad*

2019   **Silver Medal**, *51st International Chemistry Olympiad*

2019   **1st place**, *Austrian National Chemistry Olympiad*

2019   **1st place at the students' competition**, *University of Vienna*

2019   **Silver Medal**, *53rd International Mendeleev Chemistry Olympiad*

2018   **Bronze Medal**, *50th International Chemistry Olympiad*

2018   **Silver Medal**, *44th Austrian National Chemistry Olympiad*

2018   **Silver Medal**, *European Science Olympiad*

2018   **Audience Award & 2nd place students' competition**, *University of Vienna*

Conferences and Research

2024   **Chemical Science Journal Poster Prize**, *Royal Society of Chemistry. Awarded to top poster presentation at Faraday Discussions, Oxford, UK.*

2024   **Physical Chemistry Chemical Physics Journal Poster Prize**, *Royal Society of Chemistry. Awarded to top poster presentation at Chemical Compound Space Conference (CCSC), Heidelberg, Germany.*

2020   **Laureate for the Dr. Hans Riegel Fachpreis (1st place in Chemistry)**, *University of Vienna / Kaiserschild Foundation. Awarded to top high school research projects in chemistry in Germany and Austria.*

2020   **Laureate for the school award**, *IST Austria (ISTA). Awarded to top high school research projects in STEM in Austria.*

2020   **Agnes-Ruis-Prize**, *Society of Austrian Chemists (GÖCH). Awarded to best expeimental research high school project in chemistry in Austria.*

Outreach

International Olympiads (IChO)
- Exam Co-Author for the 55th IChO 2023 in Switzerland: drafted, created and corrected 340+ exams (2021-2023)
- Contributed chapter for the book "10 Things You Must Know About IChO" (2023)

Women in Natural Sciences at ETH Zurich (WiNS)
- Association representing all female researchers in Chemistry, Chemical Engineering, Biology, Physics and Material Science at ETHZ
- Webmaster (2022-2024) and first-ever Student Representative (2021-2022): building website and backend from the bottom-up

Mentoring
- Mentor at the first-ever mentoring program of WiNS for undergraduate students at ETHZ (2023-2024)
- Mentor in Organic and Physical Chemistry for the Austrian National Chemistry Olympiad (2021 and 2024). 1-to-1 mentoring for top students in national and international competition.
- Leading a team of five teaching assistants: creating course contents, lecture script, exercise classes for 180+ undergraduate students (2023)
- Co-supervision of undergraduate student Huixuan Guo during internship at EPFL (Jun-Jul 2024), resulting in a poster presentation at the AI4Mat 2024 Workshop in Vienna

Teaching

2023	**Inorganic Chemistry I**, *Head Teaching Assistant (5 TAs, 180+ undergraduate students)*
2022	**Inorganic Chemistry I**, *Teaching Assistant*
2022	**Physical Chemistry I - Thermodynamics**, *Teaching Assistant*
2021	**General Inorganic Chemistry I**, *Teaching Assistant*
2021, 24	**Austrian Science Olympiad**, *Tutor (Organic Chemistry)*
2018-21	**European Science Olympiad**, *Mentor (Chemistry)*

Presentations

07/2024	**Poster Presentation**, *"Toward A General Synthesis Planning Tool for Single Atom Catalysis" at the AI4Mat Workshop in Vienna, Austria and the Faraday Discussions in Data-Driven Discovery in the Chemical Sciences in Oxford, UK. Awarded with a poster prize.*
06/2024	**Oral Presentation**, *"Digital Chemistry: A Paradigm Shift" at the annual ETH Zurich Foundation donor event as the ESOP scholar representative (chosen among cohort of 200+ scholarship holders). Held in German.*
05/2024	**Poster Presentation**, *"Decoding Solid-State NMR Descriptors using Machine Learning" at the CCSC 2024 in Heidelberg, Germany. Awarded first poster prize (1st out of 60)*
04/2024	**Poster Presentation**, *"A Digital Chemistry Atlas" at the annual Meet-The-Talent Event by the ETH Zurich Foundation*
08/2023	**Poster Presentation**, *presenting my semester project "Decoding Solid-State NMR Descriptors using Machine Learning" at the SCS Fall Meeting (annual conference of the Swiss Chemical Society) as the youngest member of the group*
04/2019	**First Prize**, *Students' Competition of the University of Vienna, Topic "How Can We Save Our Climate?"*
04/2018	**Second Prize and Audience Award**, *Students' Competition of the University of Vienna, Topic "Health Out Of The Lab"*

PUBLICATIONS

Ontology-Retrieval Augmented Generation for Scientific Discovery
Andres M Bran, Alexandru Oarga, Matthew Hart, **Magdalena Lederbauer**, Philippe Schwaller
ICLR 2025 (submitted)

ChemLit-QA: A human evaluated dataset for chemistry RAG tasks
Huixuan Guo, Geemi Wellawatte, **Magdalena Lederbauer**, Anna Borisova, Matthew Hart, Marta Brucka,
Philippe Schwaller
NeurIPS 2024 Workshop ML4PS

Scientific Knowledge Graph and Ontology Generation using Open Large Language Models
Alexandru Oarga, Matthew Hart, Andres M Bran, **Magdalena Lederbauer**, Philippe Schwaller
NeurIPS 2024 Workshop FM4Science and *NeurIPS 2024 Workshop AI4Mat*

SKILLS

Programming : Python, C++, R, Git, LaTeX

Machine Learning : Deep Learning, NLP, Large Language Models (Working with API and locally, Benchmarks,
Agents), Graph Neural Networks (PyTorch Geometric, Heterogeneous GNNs)

Libraries : PyTorch, PyTorch Geometric, Tensorflow, SciKit, RDKit, DSPy, Langchain, LLamaIndex, ChromaDB

Computational Chemistry : DFT calculations (ORCA, Gaussian), semiempirical methods (GFN2-xTB)

Languages : German (Native), English (Fluent), French (Conversant)