Magdalena Lederbauer

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Education

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

- Focus Digital Chemistry, Catalysis, Chemical Engineering
- Selected into the **Excellence Scholarship & Opportunity Program** (ESOP) awarded to top 2% students
- Master's thesis at MIT (Connor W. Coley) 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* *Cambridge, MA, USA*
Supervisors: Prof. Dr. **Connor W. Coley**, Dr. Runzhong Wang
Toward structure elucidation from mass spectrometry using neural networks

03/24-07/24 **EPFL, Laboratory of Artificial Chemical Intelligence**, *Internship* *Lausanne, Switzerland*
Supervisors: Prof. Dr. **Philippe Schwaller**, Andrès M. Bran
Large Language Model Agents in Heterogeneous Single Atom Catalysis

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

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

02/23-05/23 **ETH Zurich, Copéret Group**, *Research Project* *Zurich, Switzerland*
Supervisors: Prof. Dr. **Christophe Copéret**, Dr. Zachariah Berkson
Decoding Solid-State NMR Descriptors using Machine Learning

07/20-08/20 **Leopold-Franzens-Universität**, *Internship* *Innsbruck, Austria*
Supervisors: Prof. Dr. **Hubert Huppertz**, Dr. Freia Ruegenberg
Synthesis of narrowband luminescent materials for Solid State Lighting applications

08/19 **Technical University of Vienna**, *Internship* *Vienna, Austria*
Supervisors: Prof. Dr. **Katharina Schröder**, Dr. Aitor Sainz Martinez
Synthesis and applications of ionic liquids comprising alkylmethylimidazolium-cations .

Selected Awards

2024	**Zeno Karl Schindler Foundation Master Thesis Grant**, *Merit-based excellence scholarship for master's theses in engineering disciplines. Granted CHF 12k.*
2024	**Chemical Science Journal Poster Prize**, *Royal Society of Chemistry*
2024	**Swiss-European Mobility Programme (SEMP) Scholarship**, *ETH Zurich. Granted CHF 3k.*
2024	**2nd Place & Knowledge Graph Prize**, *Worldwide LLM Hackathon for Applications in Materials Science and Chemistry*
2024	**Physical Chemistry Chemical Physics Journal Poster Prize**, *Royal Society of Chemistry*
2023	**Impact Potential Prize**, *Swiss Data Science Center (SDSC) Generative AI Hackathon*
2023	**Excellence Scholarship and Opportunity Programme (ESOP)**, *ETH Zurich. Granted CHF 36k.*
2020	**Exzellenzstipendium Ausland - Excellence Scholarship**, *Lower Austrian Society for Research Promotion. Granted 60k.*
2020	**Laureate for the Dr. Hans Riegel Fachpreis (1st place in Chemistry)**, *Universität Wien / Kaiserschild-Stiftung*
2020	**Silver Medal**, *52nd International Chemistry Olympiad*
2020	**1st place**, *Austrian National Chemistry Olympiad*
2020	**Laureate for the school award**, *IST Austria*
2020	**Laureate for GÖCH-VWA-award in Chemistry**, *Gesellschaft Österreichischer Chemiker*
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*

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)
- Mentor in Organic and Physical Chemistry for the Austrian National Chemistry Olympiad (2021)

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 of the Austrian Chemistry Olympiad (2023-present), supervising and guiding high school students in preparing for the 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*

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 the Chemical Science poster prize.*

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) by Physical Chemistry Chemical Physics (PCCP).*

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)*

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)