

# PhD in Machine Learning for Sustainable Synthesis at EPFL

We are looking for highly motivated PhD students for projects at the intersection between advanced machine learning and chemistry. We will have **multiple fully-funded positions in early 2022** (the earliest starting date is February 2022). Candidates applying are expected to begin their PhD before October 2022. Together we will create impactful methods for accelerated and sustainable chemical synthesis and discovery.

## Project background

Over the last hundred years, not much has changed how organic chemistry is conducted. In most laboratories, the current state is still trial-and-error experiments guided by human expertise acquired over decades. What if, given all the knowledge collected and expertise gained, we could develop machine learning-based assistants to accelerate the discovery of novel molecules and design sustainable routes incorporating green chemistry principles?

Although we currently observe a rise in machine learning approaches for chemical synthesis, they are only scratching the surface of what is feasible. We want to foster close collaborations with synthetic chemists, develop approaches that can be tested experimentally, and facilitate the adoption of machine learning techniques in their daily workflows.

Possible thesis topics could be reaction prediction beyond the Molecular Transformer, sustainable synthesis route planning, reaction optimisation (high-throughput experimentation/human in the loop), de novo molecule design from renewable feedstocks, and equivariant neural networks for modelling (heterogeneous) catalytic processes. Machine learning is a fast-moving field. Together we can adapt the topic to your and the labs interests.

## Your profile

- A Master degree or a four or five-year Bachelor degree in Chemistry, Chemical Engineering, Computer Science or related fields
- Motivation for working on challenging projects, passion for scientific research, and thrive for excellence

- Strong teamwork and communication skills
- Growth mindset and inclusive team culture
- English proficiency
- Programming and machine learning experience (e.g. in Python)

## Application and Selection Process

1. Send a CV and summary (1-2 pages) of previously done research projects to [philippe.schwaller@epfl.ch](mailto:philippe.schwaller@epfl.ch) with the subject "PhD in Machine Learning for Sustainable Synthesis".
2. Selected candidates will be invited first to a non-technical discussion and then in a second round to a technical interview (including a 25 minutes presentation).
3. PhD positions require acceptance to the doctoral program of Chemistry and Chemical Engineering. Becoming a PhD student at EPFL thus consists of applying at: <https://www.epfl.ch/education/phd/edch-chemistry-and-chemical-engineering/edch-how-to-apply/>. This page also contains additional administrative information on PhD positions at EPFL.

We look forward to receiving your application before **November 21, 2021**.

## Doing a PhD at EPFL

The École Polytechnique Fédérale de Lausanne (EPFL) is a world-leading university and provides an internationally recognised, collaborative and well-funded environment. QS World University Rankings, for instance, rank EPFL in the top-10 worldwide in Chemistry and Computer Science and Information Systems. With the Center for Intelligent Systems (CIS), EPFL has a platform to promote interdisciplinary research in artificial intelligence and machine learning and connect researchers from various fields.

EPFL is located in Lausanne, in the French speaking part of Switzerland (by train ~40 min to Geneva, ~2 hours to Zurich). Switzerland is a beautiful and safe country with great work-life balance and life satisfaction. Mountains and great outdoor activities (e.g. hiking, biking, sailing, and skiing) are never too far away.

As a PhD student, you are an employee entitled to 5 weeks per year of paid vacation, which have to be taken without guilt. You will receive a competitive salary (starting at ~57k USD/year). Even though there are high costs of living in Switzerland, you will live comfortably and save money for leisure activities.

There is an excellent [blog post by Mathias Payer](#) on doing a PhD at EPFL in Computer Science. Compared to the Computer Science doctoral school with 30 required ECTS course credits, the Chemistry and Chemical Engineering one only requires 12 ECTS. The courses can be taken in chemistry or machine learning depending on your interests. Summer schools and conferences are another way to obtain ECTS credits.

For more information, check out the comprehensive "[Best practices guide for doctoral studies at EPFL](#)".

All in all, PhD is a unique opportunity to dive into a specific topic, learn new skills and grow to become an expert in the field.

## Equality and Diversity

At EPFL, people from a wide range of cultural and academic backgrounds work and study together. Diversity is a strength. It requires an environment of mutual respect to allow the members of the EPFL community, individually and collectively, to achieve exceptional results.

We will encourage diversity and foster a culture of inclusion where everyone feels welcome. We will not tolerate any discrimination on grounds such as gender, sexual orientation, disability, the colour of skin, social origin, and religious affiliation.

EPFL provides support for young parents scientists and has measures to promote a balance between professional life and private/family life ([https://www.epfl.ch/about/equality/family\\_worklife/](https://www.epfl.ch/about/equality/family_worklife/)).

## Your workplace

[EPFL on Google maps](#). The lab will be situated in the CH building, close to the Rolex Learning Center.



Aerial views of the EPFL Campus. Copyright EPFL - Alain Herzog

## Contact

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Incoming Assistant Professor / NCCR Catalysis PI | February 2022

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*Apply now and become part of the story right from the start.*