

Philippe Schwaller

Ecole polytechnique fédérale de Lausanne

Laboratory of Artificial Chemical Intelligence

AI-Augmented Chemical Science through Language Models

Modern society urgently needs new medicines, sustainable materials, and efficient chemical processes. Accelerating chemical discovery has become a grand scientific challenge, as exploring the vast chemical space (estimated at 10^{60} feasible drug-like molecules) and predicting reaction pathways remain formidable tasks.

Professor Philippe Schwaller pioneers artificial intelligence to transform chemical science by treating chemistry as a language that machines can learn. His groundbreaking work encompasses data-driven computer-assisted synthesis, sample-efficient generative molecular design, and large language models (LLMs) for chemical research.

His influential Molecular Transformer taught computers to understand chemical reactions like a language, garnering over 1,000 citations and revolutionising how AI approaches chemistry. Building on this breakthrough, ChemCrow became one of the first LLM agents capable of autonomously planning and executing chemical experiments using robotic laboratories. Schwaller's team also developed a molecular design framework that creates new molecules optimised for desired properties while guaranteeing viable synthesis routes from targeted starting materials. This innovation enables practical applications such as transforming industrial waste into valuable therapeutic compounds.

Most recently, his research allows chemists to simply describe their synthetic preferences in plain English, with AI systems finding matching chemical routes – essentially enabling scientists to communicate with laboratory systems in their own language.

A defining characteristic of Schwaller's approach is the emphasis on practical applicability. Rather than developing AI methods in isolation, his research consistently bridges computational innovation with real-world chemistry, incorporating feedback from experimental chemists. His innovations establish a new paradigm where AI systems truly augment human chemists' capabilities, ultimately accelerating the discovery of life-saving drugs and sustainable materials.