

From Molecular Transformers to Quantum-Enabled Chemical Discovery AI, quantum computing, and the next digital layer for chemistry

Teodoro Laino^{1,2}

¹IBM Research Europe, Säumerstrasse 4, 8803, Rüschlikon, Switzerland

²NCCR Catalysis, Zurich, Switzerland

Over the last six years, AI has changed how we work with chemical information. We started by treating reactions as a language problem: molecules and reactions could be written, translated, predicted, and searched. This led to Molecular Transformers, at the core of the forward and procedure prediction models, as well as retrosynthesis workflows all combined in a platform named RXN for Chemistry. The same architecture was at the core of the first integration of AI-controlled laboratory automation (RoboRXN).

But chemistry is not only text. It is also spectra, structures, simulations, procedures, and experimental results. In this talk, I will show how our work moved from reaction prediction to models that connect molecules with measurements, especially IR and NMR spectra, and how this is now evolving toward multimodal models for chemistry.

I will also discuss the Swiss AI Initiative and the effort we made to build models that combine different types of chemical evidence in a reliable and reproducible way.

Finally, I will explain where quantum computing fits into this picture, not as a magic shortcut, but as part of the next digital layer for chemistry. The goal is simple: help chemists make better decisions, faster.