

Chemistry in the age of foundation models

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Chemistry faces a fundamental challenge: the space of possible molecules and materials is nearly infinite, yet discovering useful new ones requires navigating costly cycles of design, synthesis, and testing. In this talk, I will show how language models — the same technology behind modern AI assistants — can be adapted to "speak" the language of chemistry and dramatically accelerate this discovery process. We explore how small, specialized models can learn to propose novel molecules atom by atom, while respecting real-world constraints like available building blocks and preferred chemical reactions. We then turn to large language models and show how they can reason about chemistry and even assess whether a proposed synthesis is practically feasible. Finally, we present a general framework that uses language model representations to efficiently guide experimental optimization across diverse scientific domains — from drug discovery to materials science — with minimal data. Together, these advances illustrate how AI and chemistry are converging to help scientists explore chemical space faster and more creatively than ever before.