Artificial Intelligence (AI) Solutions for Computational Chemistry and Organic Chemistry Tasks

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First, we will present a deep learning model that approximates the solution of the Schrodinger equation. Focusing on parametrization for drug-like organic molecules and proteins, we have developed a single ‘universal’ model, which is highly accurate compared to reference quantum mechanical calculations at speeds 10^6 faster. These models accurately represent the underlying physical chemistry of molecules through various test cases, including chemical reactions (thermodynamics and kinetics), thermochemistry, structural optimization, and molecular dynamics simulations. The results presented in this talk will provide evidence of the universal applicability of deep learning potentials to various chemistry problems involving organic molecules.

Second, we proposed a novel ML-guided materials discovery platform that combines synergistic innovations in automated flow synthesis and automated machine learning (AutoML) method development. A software-controlled, continuous polymer synthesis platform enables rapid iterative experimental–computational cycles that result in the synthesis of hundreds of unique copolymer compositions within a multi-variable compositional space. The non-intuitive design criteria identified by ML, accomplished by exploring less than 1% of overall compositional space, upended conventional wisdom in the materials design.