

Self-driving laboratories for accelerated discovery

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In this talk, I will describe our group's interdisciplinary research towards the acceleration of molecular discovery. We focus on the discovery of small-molecule-based materials such as solid-state organic light emitting diodes and organic lasers. I will discuss artificial intelligence models for the generation of molecular candidates with particular properties, forward-synthetic space prediction methods that are amenable to automation, and Bayesian-optimization driven experimentation. In particular, for the design of organic lasers, we have designed a Chemspeed synthesis machine/HPLC-MS/laser characterization self-driving lab. I will discuss the synergies and opportunities with small-molecule drug discovery as well as process optimization. Several of the tools we have developed have been translated to these fields.