Delocalized, Asynchronous, Closed-Loop Material Discovery

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EXTENDED ABSTRACT: Contemporary materials discovery requires intricate sequences of synthesis, fabrication and functional characterization that often span multiple locations with specialized expertise and instrumentation. In our collaborative effort of the Material Accelerated Discovery of Novelty Enabled by Synthetic Systems (MADNESS) campaign, we present a cloud-based solution enabling AI-guided, asynchronous, and delocalized design–make–test-analyze cycles to integrate these workflows. We applied a building-block strategy for assembling molecular function enables automated synthesis on geographically distributed yet connected platforms, orchestrated by a central cloud platform, with the integration of an AI-based experiment planner and an in-line property characterization module to accelerate the discovery of top-performing organic solid-state laser molecules as demonstrated by the best ever thin-film device performance. Empowered by asynchronous integration of five laboratories across the globe, this workflow provides a blueprint for delocalizing – and democratizing – scientific discovery, in which we are endeavoring a global community of accelerated material discovery and self-driving laboratories based on the framework of the Acceleration Consortium at the University of Toronto. Collectively, we aim to accelerate the discovery of materials and molecules for sustainability, for health care, and for a brighter future. To demonstrate our contemporary progress, a joint effort of all AC teams as well as a pan-Canadian task force on the workflow of develop new drugs in the self-driving lab era will be introduced.

Figure 1. Delocalized materials discovery workflows over multiple sites, orchestrated by a single cloud-based application.

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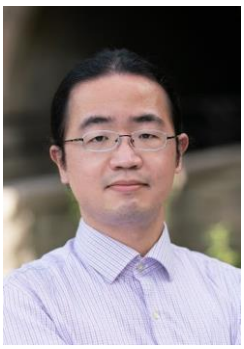
BIOGRAPHY



Dr. Han Hao is a Staff Scientist of the Acceleration Consortium at the University of Toronto. He was also a postdoctoral fellow with Prof Alán Aspuru-Guzik from the Chemistry Department at the University of Toronto. His research focus includes advanced automation and digitization of chemistry, robotics in chemistry, AI-assisted molecule design and high-throughput computations. He also works on deliverable designs and blueprints for the self-driving lab community.