

Finding Environmental-friendly Chemical Synthesis with AI and High-throughput Robotics

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Invited Talk

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Recent challenges with the environment have resulted in tremendous interest in Green Chemistry, which includes the design of chemical products and processes that reduce the use of environmentally harmful substances. Until now, finding new environmental chemical synthesis is largely a trial-and-error process, requiring trained expertise and a large amount of work. Here, we report a high-throughput process, combining AI techniques and robotic synthesis, allowing us to find a more environmentally friendly way to synthesize an existing material. The model materials in this study are to replace nitrate salts (NO_3^-), which might be responsible for algae bloom if leaked into open water, by a chloride salt (Cl^-), a natural abundant ion, in the synthesis of a metal-organic framework, Zn-HKUST-1. Our high-throughput process starts with using large language models (LLM)-based literature summary to create a database on the synthesis of Zn-HKUST-1 with NO_3^- , so that optimized concentrations of Cl^- can be suggested. Subsequently, these suggestions are tested with automatic robotic processes, increasing the speed and precision of the experiment, to find the optimal synthesis condition. Using this process, we successfully obtained MOFs (Metal Organic Frameworks) crystals from ZnCl_2 precursors. An AI-based learning process is developed, comparing the structural information of our synthesized materials with that of the database to confirm indeed the obtained MOFs are Zn-HKUST-1. This success proves that our process holds the promise to accelerate the discovery of new environmental-friendly materials in the near future.

Keywords: LLM literature synthesis, MOFs, LLM experimental verification, Green, Robotic synthesis