

Computational Design and Automation for Materials Discovery

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The increasing complexity of chemical compositions, structures, and dimensions poses significant challenges for modern materials screening and optimization through traditional trial-and-error or experimental methods. Consequently, the need to develop efficient, precise, and cost-effective approaches in materials chemistry has become paramount. To address fundamental scientific questions in materials discovery, our research group focuses on using data-driven approaches to accelerate this process.

In this presentation, I will discuss two research projects undertaken in our group. The first focuses on utilizing computational intelligence, electron diffraction, and molecular simulations to resolve the structures of poorly crystalline covalent organic frameworks (COFs). To achieve this, we implement the particle swarm optimization (PSO) algorithm, which automatically generates trial structures, allowing for comprehensive exploration of potential configurations. These models are further optimized using force field calculations and refined with experimental diffraction data to determine the most precise and accurate structures.

The second project highlights the critical role of automation tools in accelerating on-demand material synthesis and improving the materials discovery process. Specifically, we have developed an efficient methodology to speed up the discovery of polar hydrogen-bonded cocrystals. This approach combines molecular similarity-based screening, machine learning-driven cocrystal predictions, and automated synthesis techniques to streamline the assembly of cocrystals.

References:

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