Data-Enabled Synthesis Predictions for Molecules and Materials

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Abstract

Chemical and materials informatics leverages data to correlate a compound's structure with its properties, enabling the exploration of vast chemical spaces through modeling. Although this approach has the potential to reveal novel materials with desired characteristics, it frequently generates designs that cannot be synthesized, leading to demanding time and resources in experimental attempts. In this talk, I will talk about our recent efforts to build machine learning models to predict inorganic and organic synthesizability and reactivities, and their synthesis pathways. In particular, one important aspect of synthesis prediction is its explainability that can further enhance chemist understanding of synthesis to go beyond the blackbox prediction of most ML models. I will introduce some of recent endeavors to propose explainable models for inorganic and organic synthesis along with the high predictive accuracy.

References

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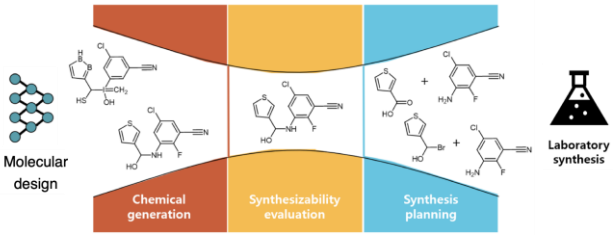

Figure 1. Chemical informatics from design to synthesis