Abstract

Discovery of a new material with desired properties is the ultimate goal of materials research. To date, a generally successful strategy has been to use chemical intuition and empirical rules to design new materials, but these conventional approaches require a significant amount of time and cost due to almost unlimited combinatorial possibilities of inorganic materials to explore in chemical space. A promising way to significantly accelerate the latter process is to incorporate all available knowledge and data to plan the synthesis of the next material. In this talk, I will present a few initial frameworks we have developed along this line to perform machine-learned density functional calculations, to predict the properties of a material (catalyst) using simple representations, and to inverse design new materials with a target property using materials deep generative model.