기계학습을 통한 고체화학 물질공간 탐색
Exploring solid-state chemical space by machine learning

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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 using simple representations, and to generate new materials for a target property using materials deep generative model.