Materials prediction using high-throughput and machine learning techniques

CHANDRAMOULI NYSHADHAM, Brigham Young Univ - Provo

The importance of designing new materials with enhanced properties is vital for mankind to prosper and meet their ever-increasing necessities. The task of searching for new and advanced materials is colossal because of the innumerable combinations of different elements. Material scientists have developed large databases of known materials over the last century. The challenge now is to use data from computer simulations to discover new materials. Here at Brigham Young University (BYU) we have built a large database of alloy simulations. High-throughput and machine learning techniques can be used to leverage the database and discover materials at a faster pace. The high-throughput technique is an intelligent way to interrogate a database for inventing new materials. Machine learning models give a computer the ability to learn about materials without being programmed explicitly. In this talk I'll give a brief overview of my three year work as a PhD student here at BYU. The talk will focus on two important topics: 1) A high-throughput technique we used to invent new materials called superalloys[1], and 2) a few machine learning techniques we are currently pursuing for faster prediction of new materials.


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