Machine-learning materials science

Miguel Marques
[1]Ruhr Universitat Bochum, Germany

miguel.marques@ruhr-uni-bochum.de

We summarize our recent attempts to discover, characterize, and understand inorganic compounds using novel machine learning approaches. We start by motivating why the search for new materials is nowadays one of the most pressing technological problems. Then we summarize our recent work in using crystal-graph attention neural networks for the prediction of materials properties. To train these networks, we developed a dataset of over 4.5 million density-functional calculations with consistent calculation parameters. Combining the data and the newly developed networks we have already scanned thousands of structural prototypes spanning a space of several billion materials and identified tens of thousands of theoretically stable compounds. We then discuss how simple, interpretable machine learning approaches can be used to understand complex material properties, such as the transition temperature of superconductors. Finally, we speculate which role machine learning will have in the future of materials science.