

Summary of Article

Predicting crystal structure by merging data mining with quantum mechanics

The summarized article deals with the concept of effectively predicting and understanding the concepts of new materials and optimizing the existing materials using the concepts of quantum mechanics.

Many times, the most critical role in material science is played by crystal structure when we must compare the material performance and basic composition. Now with the advances in computational power and the field of material science, the prediction uses lots of previous data and sets those data as a base set. Methods used by researchers rely on the representation of structural stability on basis of forces that are physically motivated such as their size difference, electronegativity etc., which led to the inefficient way to discover and analyze properties of materials.

The new methods are to merge modern tech prediction capabilities with the traditional method. For predicting crystal structure, combining quantum mechanical methods with machine learning would be helpful.

Firstly, the general approach that is taken is an information-based model called Data Mining Structure Predictor. The huge quantity of historic data is used in its development and it suggests a probable ground state structure with large-scale analysis of intermetallics. A correlation is formed using ML between materials where the range is given between 0 and 1. There are two forms of correlation and they occur between structures at different compositions.

The predicting power of DMSP is evaluated and analyzed in a general way by using cross-validation. Prediction of 3,975 compounds occurring in two or more alloys in the dataset. For a prediction to work, existing data about the alloy is removed from the dataset. Then the compound of that alloy is predicted, the composition of interest is predicted, however, currently, crystal structure with absolute certainty is not yet possible. But with the advancement in ML, we can very well get a high percentage. A more physically sound solution will be to make an energy accurate model that can be achieved by modern quantum mechanics and efficient machine learning algorithms.

Data preparation

The data for this study is obtained from the Pauline file and that database contains 28,457 entries which were determined experimentally, and it contains 2600 alloys. The study done here was restricted to metallic alloy. So several elements were removed that contain elements such as helium, carbon etc.

Calculations

The density functional theory is used in generalized gradient approximation and ab initio electronic structure calculation was carried out. By using the following calculation significant accuracy has been predicted in the model. Hence paper concludes by combining modern methods like data mining with traditional methods can greatly improve the overall accuracy of material property determination and can be used to better analyze them.

Polymer Genome

The polymergenome.com is a simple but highly sophisticated and advanced website that can be used to better study polymer it works when you enter a polymer name the algorithm then using the name predict the polymer and gives its structure, as well as its properties as well, is 2d or 3d structure. Another feature of this website is that you can simply just draw the polymer you desire and the algorithm will do the rest of the stuff for you such as give it a name show its property and its 3d structure as well as how will it interact with other elements.

Almost all modern tech contains polymer and with mass consumerism, it's a challenge to get materials cheap as well as of good quality to deliver to the customer the development of newer alloys can help overcome this challenge. And polymer genome aims to help in that initiative polymers such as polybag are used widely as well in other kinds of stuff like PVC pipe, paint, etc. polymer genome enables the easy representation of polymer.

There are both pros and cons of polymer genome

With the help of the polymer genome, we can discover new materials and can even enhance the existing ones other than that we find new properties of different polymers as well as how they interact with other materials and polymers. The website is also useful for the people who are a novice in the field of material science and wants to learn more about it as creating materials in the website by drawing is easy and can be done by almost anybody. Furthermore, this polymer genome website can gather data and ultimately help in the creation of perfect MUSE (materials Ultimate Search Engine).

There are however cons too as polymer genome still don't have sufficient data to give a result with 100% accuracy other than that it can give results of polymer that are impractical furthermore the interaction btw different polymers given by polymer genome could be wrong which can lead to potential waste of resources