Abstract

The existence of a strong magnetic material is something that needs to be sought because it can have a wide-ranging impact on daily life. However, in finding strong magnets it takes a long time when searched using the Density Functional Theory (DFT) method to find the right magnetic compositions. This is because of the many combinations that may be formed from the elements available in nature, to speed up the search process it is necessary to combine the DFT method with Machine Learning. So that science material researchers can get useful things. In this simulation, about 132 possible combinations of 2D magnetic material data will be involved, having 45 features, namely 30 atomic positions, 10 magnetic moments, total magnetic moment, fermi energy, band energy, total energy, and finally total electrons. The Machine Learning method used is the K-Nearest Neighbor method, this method was chosen because it is one part of supervised learning. Previous research using kernel ridge and neural network, the difference is in the method to be used. Machine Learning system will make the classification of strong magnets based on the characteristics of magnetic materials.

Keywords: Machine Learning, k-Nearest Neighbor, DFT