

Abstract

The discovery and design of new materials is the main goal of material science. The large amount of material data that needs to be analyzed to find new materials is a grand challenge in this field because it is taking very high computational time and resources if we calculate all of the possible structure from many material combinations using precision methods, such as Density Functional Theory (DFT). Facing these challenges, we need a system that can analyze the combination of material structures with fast performance but still maintain the precision of calculation. This is where materials informatics is present to accelerate the search for new superior material, material informatics is a new scientific field which aims to utilize information in the computational methods commonly used in scientific material. In this research, 198 combinations of two-dimensional magnetic materials of $A_2B_2X_6$ structure will be classified using support vector machine (SVM). By applying feature selection, the SVM classification model that is built can produce an accuracy and an f1-score of around 97%.