ABSTRACT

The Convolutional Neural Network (CNN) has become increasingly developed, demonstrating high accuracy and applicability across various fields. Generally, CNNs are used in image processing; however, this method is rarely applied in other areas, such as material science. With the availability of the DOSnet dataset, which stores intrinsic information about the properties of materials that is publicly accessible on the internet, we can utilize this dataset and apply the convolutional neural network method to predict one of the material characteristics, such as adsorption energy. Adsorption energy is significant in the field of material science because it determines how effectively a metallic alloy can absorb gases or radical molecules in the air. A high adsorption energy indicates that the material is of good quality and suitable for use as a catalytic filter. In this study, we utilize CNN to predict the adsorption energy value. A machine learning model based on the CNN method, using the DOSnet dataset, was able to predict the adsorption energy of a bimetallic alloy surface towards CH molecules with good accuracy. The best MAE value obtained was 0.1368 and the best RMSE value was 0.1877.

Keywords: ***machine learning | Convolutional Neural Network (CNN) | Density of States (DOS)***