Predicting melting temperature via graph neural network enhanced by transfer learning

Developing a machine learning model capable of predicting the melting points of inorganic crystals allows for rapid melting point predictions, eliminating the need for experimental synthesis and complex theoretical calculations. We improve the accuracy of these predictions on a data-scarce melting point database by applying transfer learning to a crystal graph neural network. By pretraining the model with a large atomization energy database and then transferring this learning to the melting temperature database, we achieve a satisfactory root mean squared error of 218 K. Additionally, we find that the accuracy improvement for each crystal category is significantly influenced by the physical relationships between the pretraining database and the target property. This work was published at Computational Materials Science 2023, 234, 112783.