Exploring of Salen-type Single-Molecule Magnets via Deep Learning

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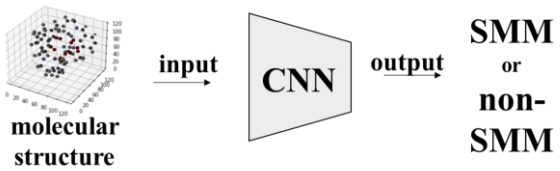
Single-molecule magnets (SMMs) are metal complexes that show bulk magnet-like magnetic relaxation behavior in a single molecule[1]. The creation of SMMs requires the construction of a coordination environment in which the spin quantum number S and anisotropic zero-field splitting D of the central metal are large. Although the discussion has conventionally been based on the symmetry of the central metal, it is necessary to find a new guideline for molecular design in order to develop new SMMs. Recently, machine learning applications in chemistry have attracted much attention, but its application to metal complexes with diverse coordination structures and electronic states has been limited[2]. The purpose of this study is to create a model to predict SMM properties from molecular structures using deep learning techniques and to investigate new molecular design guidelines.

The SMM data set was created by obtaining crystal structure and magnetic data for 400 SMM and 200 non-SMM molecules from approximately 800 Saren-type SMM papers. We generated 3D images (voxels) based on the atomic coordinates obtained from the crystal structures and used a 3D convolutional neural network (3D-CNN) to create a binary classification model that predicts whether a molecule is a SMM or non-SMM. Using this data, we trained and performed SMM prediction, which resulted in a correct prediction rate of about 70%. Using this model, we attempted to demonstrate SMM design by predicting SMM properties for salen-type metal complexes reported in our laboratory[3] and about 30,000 Schiff base-type metal complexes obtained from the Cambridge Crystal Structure Database (CSD). The present method can be used for machine learning of complex metal complexes containing transition metals and lanthanides, which have complex structures. In addition to the above, we will discuss the reliability of the prediction results and their application in the laboratory.



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