Investigation of structure-property relationships of transition metal complexes using machine learning

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Single molecule magnets have potential applications in magnetic spintronics and quantum computing. Monometallic transition metal complexes are candidate molecular magnets.
These molecules have been shown to have strong spin anisotropy below their blocking temperature. Modeling of these complexes is computationally expensive and is difficult due to coupling effects. From a dataset containing over 86,000 transition metal complexes, we investigate the performance of crystal graph neural networks (CGNN). These properties have been calculated using the TPSSh-D3BJ exchange-correlation functional. Here, we see if the CGNN can predict the metal ion charge, HOMO/LUMO gap, and other computed energies. We then compare the model performance of the CGNN against artificial neural networks which have been trained with the smooth overlap of atomic positions (SOAP) structural descriptor. A completed model can then be used in high throughput screenings to quickly filter out candidate molecular magnets. This work provides the first steps in the development of a machine-learning model for the property prediction of transition metal complexes and for single molecular magnet discovery.