Apply Machine Learning Models in Predicting Magnetic Moment of Ferrite Material

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In this work, we expand methods from computationally driven design of catalysts to designing ferrite materials. Specifically, computational material involves using density functional theory (DFT) to calculate magnetic moment as they occur over a handful of ferrite material. We would like to correlate the magnetic moment of ferrite material with electronic structures, connections, compositions and other quantities of ferrite material. All the quantities are free of computational calculations and used to set up complete user-defined features sets to fully describe the ferrite material we are interested in. We apply machine-learning algorithm to build a model that correlates the magnetic moment and defined features. We run hundreds of calculations to set up a database which will be taken as the train and test sets to be able train the machine learning model to achieve higher accuracy. Also we employ features selection algorithm in our model to be able to get rid of those redundant features and develop the feature sets in able to increase the accuracy of machine learning model in a separate way. Finally, we would like develop a model free of calculation-derived descriptors will enable the screening of vast chemical spaces with surrogate machine-learning models, which can be used to identify design rules and isolate lead molecules for further investigation.