Construction of machine learning model predicting Bader charges and application of the model to exploration of CO2 reduction electrocatalyst

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We have aimed at a construction of a machine learning model to predict electrocatalytic activities of alloys made of binary or more multiple elements for CO2 reduction. The Bader charges of the alloys are obtained by first-principles calculations, and are expected to be an important descriptor for the prediction. However, it is difficult to calculate the Bader charges when the alloys are solid solutions. This is because their crystal structures are random. In this context, we made a machine learning model that predicted the alloys' Bader charges. For making this model, we investigated the influence of the data sets for the prediction accuracy. One employed binary alloys as training data set, and used more multiple elements based alloys as the evaluation. Another is opposite. Considering their coefficients of determination of the evaluation data, former was 0.66 and latter was 0.89. The better model is expected to be useful for predicting the Bader charges of solid solution alloys in the interpolation. In this poster, we will discuss relationship of the alloys, which are visualized by t-SNE, and will mention the architecture of the machine learning model using Bader charges as descriptors and the characteristics of the visualized learning data.