Screening of Sulfide Photocatalyst Materials by Machine Learning

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Photocatalysts that is capable of producing hydrogen without CO2 emission are expected to achieve carbon neutrality. High hydrogen activity is one of the desired properties of photocatalysts, however, discovery of novel photocatalyst through experimentation alone is difficult and time-consuming because there are the large number of candidate combinations of synthesis process and materials. In this study, we used machine learning to search for novel photocatalytic materials efficiently. A Light Gradient Boosting Machine (LightGBM) machine learning model for hydrogen activity prediction was constructed using 357 sulfide experimental data on photocatalytic reaction including chemical composition, synthesis process and hydrogen activity. We applied the model exhaustively to 765 sulfides in the Inorganic Crystal Structure Database (ICSD) and extracted novel promising material candidates for sulfide photocatalyst. In addition, we will discuss the strategy of material search range expansion by introducing structural information using Graph Variational Auto-Encoder (GraphVAE) as future work.