Predicting the performance of doped hematite photoanodes incorporating the effects of lattice vibrations

Fumiya Yoshinori
Nara Intitute of Science and Technology

Photocatalytic water electrolysis is a technique that can produce hydrogen without carbon dioxide emissions.
Among photocatalysts, hematite has the advantages of being inexpensive, non-toxic, stable in water, and available in visible light.
On the other hand, it has several challenges (short hole diffusion length, low electron mobility, and slow water oxidation rate), and no practical hematite photocatalyst has yet been found.
To address these challenges, doping strategies are used.
However, there are no clear criteria for selecting the optimal dopant, and experimental trial and error continues.
Therefore, this study aims to provide new insights into dopant selection criteria by creating a dataset that combines experimental data with simulations and applying machine learning.
The experimental data to be used are those provided by the collaborators and are of doped hematite with uniform fabrication conditions.
The simulations will focus on the effect of hematite lattice vibrations on photocatalytic performance, which will be calculated using CHGNet, one of the neural network potentials, and incorporated into the predictions.
From these efforts, we aim to identify dopant selection criteria for hematite and provide design guidelines for hematite photocatalytic materials.