Photocurrent Prediction in Multi-Element-Doped Hematite Photoelectrodes Based on Machine Learning

([1]*Grad. Sch of Sci. Kobe Univ.*, [2]*Mol. Photosci. Res. Center, Kobe Univ., MS, NAIST*[3], *DSC, NAIST*[4]) ○Takuma Nishimrua,[1] Yoshitaka Kumabe,[1,2] Yosuke Harashima,[3,4] Mikiya Fujii,[3,4] Takashi Tachikawa[1,2]

Keywords: Photocatalysts; Photoelectrodes; Water Splitting; Machine Learning; Data Analysis

Photocatalytic hydrogen production reaction using sunlight is gaining attention as an environmentally friendly energy conversion method. Extensive research has been conducted to improve the photocatalytic performance of these materials. Hematite (α-Fe_2O_3), commonly known as red rust, is one of the promising photocatalytic materials for photoelectrochemical (PEC) water splitting and hydrogen production when used as a photoelectrode, owing to its abondance on Earth and nontoxicity. However, its practical application is hindered by the poor mobility and short lifetime of photogenerated carriers (a few nanometers and picoseconds, respectively). Doping the materials with additional elements is one of the most common approaches to improve their performance. In this study, we synthesized hematite photoelectrodes with various compositions and collected analytical data including Raman spectra, UV-vis transmittance spectra, and X-ray diffraction (XRD) patterns. Regression models based on a two-step LASSO method were developed to predict the photocurrent of hematite photoelectrodes using their elemental information and analytical data as explanatory variables.

Figure 1a shows the results of prediction from the two-step LASSO model using various combinations of descriptors. The regression model using elemental features and Raman spectra exhibited the highest prediction accuracy. This indicates that the photocatalytic performance (photocurrent) of hematite photoelectrodes can be explained by their elemental properties and vibrational information. Data analysis revealed that most correlation coefficients between the selected Raman signal intensities and photocurrent were negative (Figure 1b). This result implies that the reduced polarization changes of metal-oxygen bonds and the subsequent concentration of carriers on the reactive metal centers enhance the progression of PEC water splitting reaction.

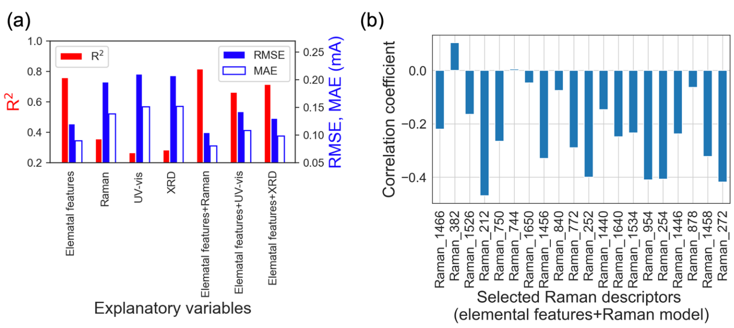

Figure 1 a. Results of prediction by a two-step LASSO regression using various types of descriptors. **b**. Correlation coefficients between selected Raman descriptors and the target photocurrent.

© The Chemical Society of Japan