Prediction of photocurrent density of various photoanodes using machine learning with feature extraction from analytical data.

([1]*Chuo University*) ○Yuya Nagai,[1] Zhenhua Pan,[1] Kenji Katayama[1]

Keywords: Machine learning, Photoanode, Photocurrent

Photoanodes are promising for solar-driven hydrogen evolution, yet their performance (photocurrent) varies despite identical preparation conditions. This suggests that the unidentified factors could affect the photocurrent of the photoanodes. To clarify the factors, we have developed a scheme to predict the material performance using machine learning (ML) from analytical data, including X-ray diffraction (XRD), Raman spectroscopy, UV/Vis absorption spectroscopy, and photoelectrochemical impedance spectroscopy (PEIS). The analytical data provided features, such as peak intensities or positions, which were used to predict photocurrent values. Then, the ML process identified the dominant factors for performance. This scheme was applied to hematite and bismuth vanadate photoanodes.[1,2] Additionally, we adjusted the operational parameter for the sample preparation based on the dominant factors through ML to enhance the photoanode activity.[3]

In our previous studies, we were unable to determine the contributions of the dominant descriptors to the performance because we used various ML methods. In addition, the use of multiple ML functions could negatively impact the robustness of our scheme when applied to various material data with target values. To address these issues, we have developed a comprehensive and robust approach that encompasses data preprocessing, ML computations, descriptor selection, and importance analysis of the dominant descriptors. The accompanying figure illustrates our recent ML methodology. In this presentation, we explain the calculation scheme and present the results of its application to hematite, bismuth vanadate, and various photoanodes.

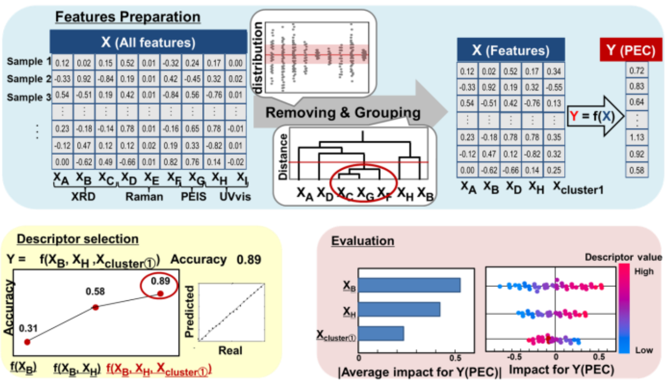

Figure. Overall ML scheme for descriptor selection and contribution analysis are shown.

1) Y. Nagai, et al. *The Analyst*, **2022**, *147*, 1313. 2) K. Kobayashi, et al. *J. Photochem. Photobiol. Chem.*, **2023**, *440*, 114651. 3) T. Idei, et al. *ACS Appl. Mater. Interfaces*, **2023**, *15*, 55644.