

Neural Network-Based Analysis of the Correlations Between Photoelectrode Performance, Microscopic Images, and UV-Vis Spectra for BiVO₄ Photoanode Electrodes

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We could predict current-voltage (J-V) curves via the convolutional neural network (cNN) model, representing the photoelectrochemical (PEC) performance of photoelectrodes, using only scanning electron microscopy (SEM) images.^[1] This research suggests that nano-structure of photocatalytic materials has a crucial factor for determination of the PEC performance. In another study on the correlation between the photocatalytic materials and its analytical data in a machine learning (ML) model,^[2] it was suggested that a specific spectral region in the UV-Vis spectrum had a strong correlation to the PEC performance, indicating the UV-Vis spectrum includes some structural information.^[3] Thus, in this study, we studied the correlation between the nanostructure in the SEM images and UV-Vis for bismuth vanadate (BiVO₄) photoanodes.

We prepared 26 samples, and they were measured with SEM in various magnifications with two different modes (SEI, BEI). We used the SEM images as input data and UV-Vis (35 points in the range of 330-500 nm) were predicted as output data using cNN. A combination of BEI and SEI images with the magnification of 10,000 provided the best prediction with >90% curve match ratio. (Figure) This result suggests that nano-structure information included in the UV-Vis spectrum can predict the PEC performance (J-V curves), and we are working on this.

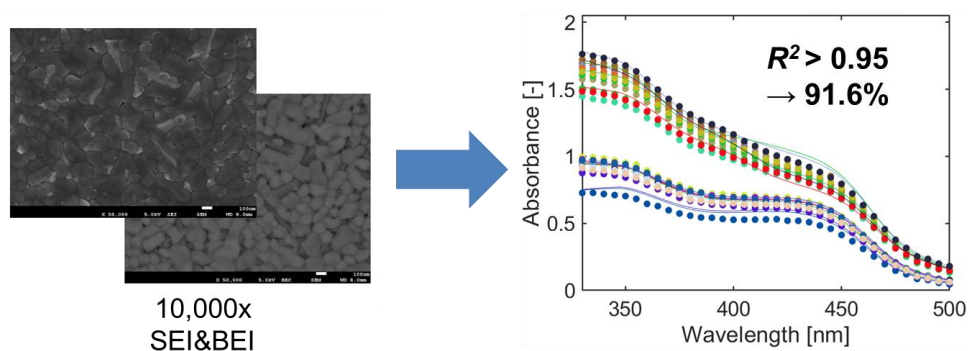


Figure The scheme of this research is provided. A combination of SEM images (SEI and BEI, x10,000) showed 91.6% prediction accuracy for the UV-Vis spectrum.

1) Y. Hayashi et.al, *J. Mater. Chem. A*, **2023**, 11, 22522-22532. 2) Y. Nagai et.al, *Analyst*, **2022**, 147, 1313-1320. 3) M. Tajima et. al, *Analyst*, **2024**, 149, 4193-4207.