Photocatalyst process informatics integrating experiment, simulation, and machine learning

Masatake Mizukami
Nara Institute of Science and Technology

It is known that photocatalyst performance varies depending on changes in the formation of products and oxygen defects in the products via calcination processes, namely heating rates, calcination temperatures, and calcination times. Recently, performance improvement by impurity substitution and understanding of its mechanism have been studied, making it necessary to consider the impurity substitution amount. It is essential to quantitatively control these factors to maximize photocatalytic performance, while these factors are difficult to control due to complex dependence of each factor, and this complexity hinders understanding of the mechanism. The present research quantifies these factors using dynamic Monte Carlo simulations, and combines the simulations with a machine learning model to predict the hydrogen evolution reaction rate. The quantified factors are used in a linear regression model as a prediction model for photocatalyst performance, and experimental results are trained to determine the model parameters including those of dynamic Monte Carlo simulation. The prediction model is employed to predict the optimum calcination process and the maximum photocatalyst performance. This approach enables the determination of the contribution of each factor to photocatalyst performance. The quantitative understanding of these contributions provides valuable insights for rational design of high-performance photocatalysts and advances the field toward more systematic optimization strategies.