Construction of cyber physical loop including dynamic Monte Carlo simulation and Application to SrTiO3 photocatalyst performance

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Searching for suitable experimental conditions for chemical synthesis is important to achieve good physical properties. Recently, with the improvement of computer performance, machine learning has been utilized to search for experimental conditions, but the large number of data points are required to improve the accuracy of machine learning. In the field of theoretical chemistry, first-principles calculations are developed to predict physical properties. We have constructed a cyber-physical loop that uses dynamic Monte Carlo simulations of chemical reactions with the results of first-principles calculations. The dynamic Monte Carlo simulation generates the amount of products and defects as features that directly influence the target variable. This is expected to provide better prediction accuracy with fewer experimental data points, since it takes into account the reasonable chemical reaction process is considered. To demonstrate the effectiveness of this method, it is applied to the photocatalytic reaction rate of SrTiO3.