Data assimilation of perovskite-type metal oxides' band gaps obtained by first-principles calculations and experiments

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We have aimed at construction of a data assimilation model for exploratively predicting experimental band gaps of perovskite-type meal oxides with few additional experiments. This is because the band gaps are properties of importance to design the materials' function such as photocatalysis. First-principles calculation is a potent tool to estimate the band gaps without time-consuming experiments, and thereby there are open databases in which the estimated band gaps are enormously stored. However, the calculation suffers from underestimating the band gap values compared to the experimental values. To address this issue, we have applied a data assimilation technique to the band gap prediction. Our concept is briefly explained as follows. First, using a machine learning technique, we make a mathematical model that well reproduces the trend of the band gaps estimated by the computation. Afterward, we make the mathematical model correspond to another model that reproduces the experimental values. The finally constructed model is expected to predict accurate band gaps not listed in experimental data sets without enormous additional experiments. In this poster, we will discuss what machine learning model is better for the data assimilation.