Exploring P-type oxide semiconductor photocatalysts using machine learning potentials

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Water splitting and CO2 reduction using photoelectrochemical cells composed of p-type and n-type semiconductors have attracted attention in terms of artificial photosynthesis. Most metal oxides are preferred as semiconductors for photoelectrochemical cells because of their chemical stability. However, most metal oxides have n-type semiconductor properties and few have p-type semiconductor properties. The development of new metal oxides with p-type semiconductor properties and materials design methods for their high performance are important for achieving highly efficient artificial photosynthesis.A method to classify p/n-type semiconductors using first-principles calculation results with energy and bandgap when hydrogen is doped in the crystal structure has been reported, but it has the problem of requiring a large amount of calculation time. Also, various doping experiments have been conducted to improve the carrier mobility of existing p-type semiconductors, but it is difficult to screen them comprehensively.In this presentation, we propose a new method for p/n-type classification by obtaining features focused on the carrier generation mechanism in semiconductors. We first demonstrated this method using first-principles calculations, and then, we examined the method using machine learning potential.