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The Effect of Co-catalyst on Water-splitting Photocatalyst: A DFT Analysis MIZUNO KAHARU, KOICHI YAMASHITA, Department of Chemical System Engineering, Graduate School of Engineering, the University of Tokyo and JST, CREST — Water splitting photocatalyst is getting wide attention due to their ability to produce H_2 by utilizing solar energy. One of the promising way to boost its efficiency is to load co-catalysts such as noble metal nanoparticles on the photocatalyst. Co-catalysts are believed to separate photogenerated electrons and holes by forming a Schottky barrier at the metal-semiconductor interface, at which O_2 and H_2 evolution reaction (OER, HER) are thought to occur. Nevertheless, the details of reactive sites and reaction mechanism are still not clear due to the difficulty in detecting OER and HER. In our research, we aimed to elucidate the relations between geometrical and electronic features of co-catalysts and to clarify the absorption structure of water on the photocatalyst by means of first-principles calculations. We picked up $Pt/SrTiO_3$ as a subject, well known cases, and found the changes in charge density difference and band structure according to the place of co-catalyst. We will also investigate the dependence of water adsorption energy on the absorption site and the role of co-catalysts in HER by analyzing the changes in electronic structures by the absorption of water on the surface.

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