Computational analysis of molecule-driven shape control of metal co-catalysts

이상헌†
이화여자대학교
(sang@ewha.ac.kr†)

Optimization of the metal co-catalyst structure is indispensable to improving the efficiency of the photocatalyst. By performing a series of experiments and simulations, we demonstrate the effect of selective particle shape control of metal co-catalysts (Au, Ag, Cu and Pt) by the CO_2 induced gas ligands (CO_2 and CO) on photocatalytic CO_2 conversion activity and selectivity. In particular, proper interaction between the gas ligand and the metal co-catalyst surface, realized by strengthening the metal-CO_2 adsorption and weakening the metal-CO adsorption, is identified as essential factor for increasing the CO2 conversion activity. Pt and Cu, which exhibit relatively strong interaction with gas molecules, have the improved photocatalytic CO2 conversion activity when grown under CO_2. In contrast, Au and Ag, which exhibit relatively weak interaction with gas molecules, have the enhanced photocatalytic CO_2 conversion activity when grown under CO. This systematic understanding can be a guideline for controlling the metal co-catalyst surface structure and will maximize the photocatalytic selectivity of the CO2 conversion.