First-Principles Study of Ag-Cu_2O Heterostructure for Selective CO Production by Electrochemical CO_2 Reduction

임새미, 이상헌†
이화여자대학교
(sang@ewha.ac.kr†)

To mitigate the concern over the CO_2 mediated global warming, there is an urgent need to develop a chemical process with eco-friendliness and energy efficiency for converting CO_2 into useful chemicals. The selectivity and energy usage of the overall CO_2 reduction system is determined by the degree of interaction between the catalyst surface and the reaction intermediates. In this study, we assess whether the catalyst structure design of placing Ag surface layers on a Cu_2O substrate is an effective way to improve the catalytic activity of Ag for electrochemical CO_2 to CO conversion by performing a series of first-principles calculations. We obtain realistic structural models of the Ag surfaces on Cu_2O by changing the Cu_2O surface termination and the number of Ag monolayer sheets. We identify the key factors that improve the CO production activity while reducing the energy consumption. Our calculation results demonstrate a significant catalytic activity improvement of Ag monolayer on the Cu_2O due to the ligand effect. This study provides an important insight into the strategy of further optimization of the catalyst performance through alloying and nanostructuring.