DFT Comparison the Performance of Pd10Sn5 and Pd10Ag5 Electrocatalyst for Reduction of CO2

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Abstract

CO2 electrocatalysis as a hydrocarbon is a promising means of achieving economical CO2-mediated hydrogen energy cycling. Hydrocarbons are renewable hydrogen storage materials. The development of reliable metal alloy electrocatalysts is an urgent but challenging task associated with such systems, although there is still a lack of precise reaction mechanism design. In this study, the performance of Pd10Ag5 alloy nanoparticles (NPs) and Pd10Sn5 alloy nanoparticles (NPs) on the electrocatalytic reaction of CO2 was compare. The kinetic and density functional theory (DFT) calculations show that the selectivity of the Pd-based bimetallic catalyst to the C2 product is greater than that of C1, and the stability of Pd10Ag5 is better and less affected by the reaction environment. However, the catalytic performance of the Pd10Sn5 electrocatalyst in the liquid phase is the best. The insight obtained from the calculations is used to develop criteria for identifying new and improved catalysts for electrochemical CO2 reduction.

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