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Abstract

The introduction of stabilizing elements, such as Au, has been recognized as an effective approach to increasing the durability of Pt electrocatalysts toward oxygen reduction reaction (ORR). However, significant tensile strain involved in this system leads to an undesirable decrease of its intrinsic ORR activity as compared to the native Pt, due to a ~3.8% tensile strain of Pt layer on Au core. In this work, we demonstrate that for a core-shell structured Pt monolayer on nanoporous gold (NPG), electrochemical potential-cycling can induce PtAu surface alloy formation, which results in unexpected improvement of its ORR activity. Theoretical calculations suggest that PtAu surface alloys possess more suitable configurations that give relatively low changes of free energy for the corresponding overpotential-determining step during ORR relative to Pt monolayer on Au. The improved ORR performance and high utilization of Pt make the nanoporous metal-based electrodes promising for green energy technologies.

Keywords:

Nanoporous gold; PtAu surface alloys; Oxygen reduction reaction; Density functional theory calculations