First-Principles Calculations for the Mechanism of Sulfur Poisoning on Ni-based Bimetallic Alloys

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Fuel cell is a promising technology to alternate the route for future power generation. In terms of cost, high efficiency, low pollution, and fuel flexibility, solid oxide fuel cell (SOFC) has many desirable advantages compared to other types of fuel cells. Among the components of SOFC, the metal catalysts supported by oxides on the anode play an important role on the cell performance. A Ni catalyst supported on yttria-stabilized zirconia (YSZ) has been usually exploited as the anode of SOFC due to its higher catalytic activity and lower cost than other metals. However, the Ni catalyst could be deactivated by sulfur containing compounds. The development of sulfur-tolerant materials is therefore an urgent task for SOFC research. In this study, we investigated the mechanism of sulfur poisoning on Ni-based bimetallic alloys (Ag/Ni, Au/Ni, Cu/Ni, Pd/Ni, Pt/Ni, Rh/Ni). We then suggested a way of alleviating sulfur deposition in comparison to the pure Ni catalysts. Our results will be helpful to design sulfur-tolerant electrode materials in SOFC.