DFT Study for Mechanistic Investigation of Sulfur Poisoning on Ni and Ni-based Alloys Supported on YSZ

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Solid oxide fuel cell (SOFC) has advantages compared to other types of fuel cells due to low cost, high efficiency and low pollution emissions. Ni catalyst has been conventionally used as the anode of SOFC. However, the sulfur contained feedstock can induce the deactivation of catalytic activity. To prevent anode deactivation, we should develop the sulfur-tolerance catalysts with understanding the reaction mechanism of sulfur poisoning. In this study, we performed density functional theory (DFT) calculations to investigate the mechanism of sulfur poisoning on Ni-based catalysts supported on yttria-stabilized zirconia (YSZ). Firstly, to identify the alloying effects, we carefully studied the sulfur poisoning mechanism on Ni(111) and Ni-based alloy catalysts (Cu/Ni, Rh/Ni, Pt/Ni, Ag/Ni, Pd/Ni, Au/Ni). Then, we carried out the same procedure on Ni and Ni-based alloys/YSZ to examine the role of support and under-coordinated sites. On the basis of the mechanistic information on sulfur poisoning, lastly, we suggested the noble strategy for designing the anode material with high sulfur-tolerance.