Improving Sulfur Poisoning Resistance of Ni Anode Catalyst in Solid Oxide Fuel Cell: A DFT Study

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Solid oxide fuel cells (SOFCs) are efficient energy conversion devices that convert chemical fuels such as hydrocarbons directly into electricity. At the anode, the oxidation reaction of the fuel occurs. These fuels contain impurities including hydrogen sulfide, which can strongly contaminate the electrodes, block the active sites, and thus degrade SOFC performance. Although removing sulfur impurities in the fuel is the most desirable method, it is inefficient because it takes a lot of time and cost. Therefore, developing a catalyst with high sulfur-poisoning resistance can be an accessible strategy. In this study, to improve the Ni/YSZ catalyst, which is conventionally used the anode materials of SOFC, we investigated the mechanism of sulfur poisoning behavior on various Ni-based alloy surfaces depending on the surface facets by using DFT calculations. Based on the results, we found that the effect of transition metal alloying into Ni on the adsorptions of intermediates and the activation barriers in the H_2S decomposition reaction, and the way of alleviating the sulfur deposition. Our DFT results will provide useful insights into the design of sulfur-tolerant SOFC anode materials.