A First-Principle Study of Sulfur Poisoning on Ni-based Bimetallic Alloys

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Rapid increase of worldwide demand for hydrocarbon fuels, thereby vast amounts of emission of greenhouse gas motivate to develop environmentally friendly alternatives to fossil fuels. Solid oxide electrolyzer cell (SOEC), which operates in the reverse mode of conventional solid oxide fuel cell (SOFC), is a promising candidates to alternate route for solving the current energy issues. Among the components of SOEC, the metal catalysts supported by oxides on the cathode play an important role on its performance through the three reactions; electrolytic half reactions of H2O and CO2 and reverse water gas shift reaction. A Ni catalyst supported on YSZ is conventionally used as the cathode of a SOEC due to its higher catalytic activity and lower cost than other pure metals. However, it is commonly known that Ni catalysts can be deactivated by sulfur containing compounds. Therefore, the development of sulfur-tolerant materials are an urgent task for SOEC research. In this study, we investigated the mechanism of sulfur poisoning on Ni-based bimetallic alloys from sulfur-containing compounds. Based on our results, we suggested a way of alleviating sulfur deposition in comparison to the pure Ni catalysts. Our results will be helpful to design sulfur-tolerant cathode materials in SOEC.