Density Functional Theory Based Screening of Binary Transition Metal Catalysts for Co-Electrolysis of Steam and Carbon Dioxide

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Rapid increase of worldwide demand for hydrocarbon fuels, and accordingly vast amounts of emission of greenhouse gas motivate us to develop environmentally friendly alternatives to fossil fuels. Syngas produced via high-temperature co-electrolysis of steam and carbon dioxide can be an alternative route to solve the current energy issues. The co-electrolysis utilizes renewable energy or nuclear powered-sources to simultaneously electrolyze steam and CO_2 at high temperature for efficient large-scale syngas production. Solid oxide electrolyzer cell (SOEC) is a device to achieve the co-electrolysis, which operates in the reverse mode of conventional solid oxide fuel cell (SOFC). Using Density functional theory (DFT) calculations, we aim to search a wide range of binary transition metals with high catalytic activities for SOEC fuel electrode. Firstly, we identified the stability of binary metal alloys and a simple descriptor which can easily predict the catalytic activity. Based on these criteria, we performed high-throughput screening to suggest the promising candidates. Our DFT based screening will be helpful to experimentalists to design high-performance SOEC fuel electrode.