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

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Carbon dioxide emitted by burning carbon-based fossil fuels is one of the main causes of global warming and climate changes. The high temperature steam/CO_2 co-electrolysis has been regarded as an alternative solution to reduce CO_2 by converting the feeding gases to syngas. Moreover, the product gases can be main resources in useful chemical reactions such as Fischer-Tropsch process. Conventionally, the monometallic Ni has been used for the fuel electrode material of high temperature solid oxide electrolysis cells (SOEC) due to its good electrical conductivity and low cost. However, Ni catalyst still has several issues for high performance SOEC such as high overpotential and low poisoning resistance. Therefore, in this study, we performed the computational screening of transition metal catalyst to totally or partially replace the Ni catalyst using density functional theory (DFT) calculations. Based on our results, we found that Fe- or Co-doped Ni bimetallic catalysts would be good candidate materials.