Exploring New Metal Catalysts with High Catalytic Activity on SOEC Electrode for High Temperature Steam/CO_2 Co-electrolysis

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Introduction

As an increase in oil price and the depletion of oil reserves, fossil fuel-based energy production will not be able to satisfy the constantly increasing energy demand. Instead, hydrogen energy becomes a promising source as an alternative to the fossil fuel-centered energy systems. However, conversion to a hydrogen-based infrastructure requires a lot of efforts. The co-electrolysis of steam/carbon dioxide can produce syngas without modifying existing infrastructure and reduce emission of greenhouse gases and usage of fossil fuels [1]. Although Ni/YSZ has been used for the electrode material of high temperature solid oxide electrolyzer cell (SOEC) with the high electrical conductivity and low cost, it still remains several problems to achieve high performance such as high overpotential and low poisoning tolerance [2].

In this study, we performed the computational screening of transition metal catalysts for SOEC electrode using density functional theory (DFT) calculations with considering electrochemical reactions. Based on our results, we found several promising candidates which can be the alternative catalysts to nickel.

Results and Discussion

We calculated the reaction energies and activation energies of CO_2/H_2O dissociation reaction on 11 transition metals on the basis of oxygen spillover mechanism. We found the Brønsted-Evans-Polanyi (BEP) relationship between activation energies and reaction energies as well as scaling relation between the adsorbates on metal surfaces. Among the adsorption energies we considered, $E_{ads}(CO)/E_{ads}(O)$ and $E_{ads}(H)/E_{ads}(O)$ can be used as the promising key descriptors to predict the activity for CO_2 and H_2O electrolysis, respectively.

Furthermore, microkinetic analysis was performed to obtain turnover frequencies (TOF) for CO_2 and H_2O dissociation reactions on the transition metals. At the operating conditions of 1023 K and 1.3 applied voltage, the feed gas contains 90% (CO_2 + H_2O) and 10% (CO + H_2) [3]. As shown in Fig. 1, Fe, Ru and Co are placed near the top of volcano plot, which is suggested to be good candidates for SOEC catalysts.

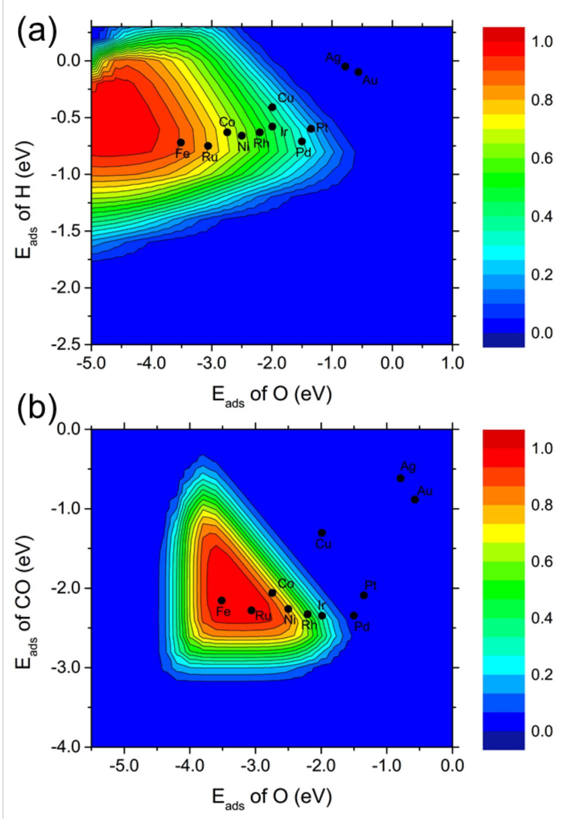

Fig. 1 Normalized activities of (a) H_2O electrolysis and (b) CO_2 electrolysis on various transition metal surfaces. The calculated activities from the microkinetic model are expressed as ln(TOF).

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