Computational screening of rutile oxide based electrocatalysts for highly selective and active hydrogen peroxide generation

이승민, 김유진, 정관영, 곽상규†
울산과학기술원
(skkwak@unist.ac.kr†)

Hydrogen peroxide (H_2O_2) is an essential chemical widely used in the applications such as wastewater purification. On the industrial scale, H_2O_2 is mainly produced by anthraquinone oxidation, which requires significant energy consumption owing to multistep process and generates organic by-products. Photoelectrochemical oxidation of water can be one of the alternative ways to produce H_2O_2 due to solar energy-induced sustainable and environment-friendly process. However, to efficiently produce H_2O_2 through water oxidation, we should control the competitive reaction, which is known as oxygen evolution reaction (OER). Thus, in this work, computational screening was conducted in the wide range of rutile oxides (MO_2) considering various conditions of the surface to discriminate OER but promote the H_2O_2 production. To elucidate selectivity and activity of the considered MO_2, the conventional volcano approach was employed based on the adsorption free energy calculation. Further, the scaling relation results provide valuable insight into identifying selective and active candidate materials and trends among MO_2 for the H_2O_2 generation reaction.