Density functional theory study of selective electrochemical ozone production on SiO_x-deposited Ni-Sb-SnO_2

정석현, 김석, 한정우†, 조강우
포스텍
(jwhan@postech.ac.kr†)

Electrochemical ozone production via six-electron water oxidation reaction (6e-WOR) represents an attractive route for efficiently generating ozone. To date, Ni-Sb-SnO_2 (NSS) has been intensively investigated as a representative ozone evolution reaction (OZER) catalyst. However, the desired OZER inevitably competes with 4e-WOR oxygen evolution reaction (OER), which limits its efficiency and durability. In this study, using density functional theory (DFT) calculations, silicon oxide coatings (SiO_x) is are introduced onto NSS to tune the selectivity of 6e-WOR. Theoretical analyses reveal that significantly promoted OZER selectivity was attributed to the surface modification via SiO_x deposition. SiO_x on NSS effectively controls the adsorption properties of intermediates and modifies electronic properties of the electrode. Our theoretical analysisresults will provide useful guidance for catalyst design to improve OZER catalytic efficiency.