

Theoretical Study on the Electronic Structures and O₂ Reduction for Rutile RuO₂/CrO₂(110) Heterostructures

임형용, 김수환, 박성오, 곽상규[†]
울산과학기술원
(skkwak@unist.ac.kr[†])

The sluggish kinetics of oxygen reduction reaction (ORR) has been a key problem impeding the commercialization of the energy converting devices such as metal-air batteries and fuel cells. It is of significant importance to controllably modify the electronic structure of the electrocatalyst surface. Thus, we targeted to study the heterojunction system composed of two different rutile metal oxides (MO₂; M = Ti, Sn, Ru, Cr, V) to enhance the ORR activity of the MO₂ surface with inferior ORR activity using the density functional theory calculation employing Hubbard U parameters (DFT+U). The oxygen adsorption energies of 4-layered MO₂ heterostructures were screened to find out the heterostructure achieving the favorable oxygen adsorption, the rate-determining step of the ORR. It was found that the RuO₂/CrO₂(110) heterostructure highly improved the oxygen adsorption. The improved oxygen adsorption was originated from a strong electron density accumulation in the interface, which could create strong internal electric field enhancing the catalytic activity of the surface. Notably, this phenomenon was also observed in further analysis of the 6,8-layered RuO₂/CrO₂(110) heterostructure.