

Hematene for the oxygen evolution reaction: oxygen vacancy role

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Abstract Using density functional theory (DFT) calculations, the catalytic activity of a recent member of two-dimensional (2D) materials, hematene (α -Fe₂O₃ monolayer), has been studied for oxygen evolution reactions (OER). The stability and electronic structure of two experimentally faceted sheets of hematene, (001) with anti-ferromagnetic and ferromagnetic coupling, was investigated. It was found that the isolation of bulk hematite to hematene leads to a surface energy of 1.03 J/m² which is much higher than those for layered materials and indicates the non-van der Waals character of the exfoliated materials. The electronic structure calculations indicate that (001) facets of hematene with anti-ferromagnetic and ferromagnetic coupling are semiconducting monolayer with a band gap of about 1.06 eV and 0.6 eV, respectively. We also studied the relationship between the experimentally observed facets and their OER catalytic reactivity. In comparison to the bulk surface, hematene has a smaller OER overpotential (1.59 eV) due to the high density of surface-active sites and modified electronic structure. The presence of oxygen vacancy creates a greater number of active sites for enhancing the electrochemical OER activity and reduces the OER potential barrier from 1.39 eV to 1.28 eV. Our theoretical and experimental results provide insights for optimizing the electrocatalytic character of the naturally occurring materials for OER application.