Enhanced Photoelectrochemical Properties of Fe-TiO₂ Nanotube Films: A Combined Experimental and Theoretical Study

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Fe-doped TiO₂ nanotube array (Fe-TiO₂ TNTA) films are produced by a simple and facile anodization method on Ti foil substrates. The Fe-doped TNTA films were characterized by SEM, Raman, XPS and UV-vis spectrum. The result showed that the absorption edge generated bathochromic shift. Raman and XPS reveal that Ti⁴⁺ ions were uniformly substituted by Fe³⁺ ions or Ti-O-Fe bonds. After comparing different Fe³⁺ ions concentrations, 0.1M Fe-doped TiO₂ samples exhibit the highest photocurrent value, indicating super photoelectrochemical activity. The difference between the photocathodic protection properties of TNTA films and Fe-doped TNTA films is also investigated. The density functional theory (DFT) calculation is carried out to confirm the effects of the Fe³⁺ ions on the absorption edge redshift and the bandgap changes.

Keywords: TiO₂ nanotube arrays; Fe-doped; Photoelectrochemical; EIS; DFT calculations;

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