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Ti-suboxides structures for water splitting

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The photo-electro-chemical (PEC) splitting of water requires semiconductors with minimum energy gap of 1.23 eV and with conduction and valence bands overlapping the oxidation of H_2O and the reduction of H^+ respectively. Titania (TiO_2) has been extensively investigated as photo-anode for PEC water splitting due to its suitable band-edge position, chemical resistance, environmental suitability and low cost. The main limitations of stoichiometric TiO_2 are its wide band gap (3.2 eV) and electron-hole recombination. Previous work on Ti-suboxides has shown that is possible to control the extent of oxygen vacancies and the electrical conductivity can be altered from 10^{-9} S/m (TiO_2) to 10^4-10^5 S/m (Magnéli phases). It has also been shown that the oxygen vacancies in the structure of Ti-suboxides increase the carriers' density and thus the photocurrent efficiency.

Other parameters to increase the efficiency is to increase the surface area and use composites structures (i.e. thin films on ferroelectrics) to enhance electron-hole separation. The approach of this work is investigating both parameters and measuring the photocurrent efficiency. TiO_2 nanotubes were grown on a Ti mesh that were then heat-threated in a reducing atmosphere introducing oxygen vacancies in the structure. The nanotubes on a Ti mesh offer very high surface area. Thin Ti-suboxides films were also investigated on a ferroelectric substrate. The field of the ferroelectric enhances the electron-hole separation. The PEC measurements were performed in a three electrode system using CSE as reference electrode and Pt wire as counter electrode. Linear voltage sweeps were collected in 1M KOH electrolyte under five wavelengths (368, 455, 525, 590 and 618 nm).

Keywords: Ti-suboxides, water splitting

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