Short Communication

Synthesis and First-principle Calculation of TiO₂ Rutile Nanowire Electrodes for Dye-sensitized Solar Cells

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In this paper, a TiO₂ nanowire film synthesized via a hydrothermal method was prepared as a photoanode for dye-sensitized solar cells (DSSCs). The synthesized TiO₂ nanowires were characterized by transmission electron microscopy and X-ray diffraction. The TiO₂ nanowire film greatly improved the efficiency of the DSSC owing to the rapid interfacial electron transport in the one-dimensional TiO₂ nanowires. The light absorption and interfacial electron transport, which play important roles in the efficiency of DSSCs, were investigated by UV-vis absorption spectroscopy and electrochemical impedance spectroscopy. The energy band structure and electron density of states of the rutile nanowire were calculated using a first-principles method and compared to bulk anatase and rutile TiO₂ phases. The band gap of the rutile TiO₂ nanowire was found to be less than that of anatase TiO₂ by 0.6 eV. Further calculations using GGA+U yielded a similar band gap reduction. In addition to the redshift of the absorption edge originating from the smaller band gap, the larger surface area of the TiO₂ nanowire compared to the bulk material is expected to facilitate the migration of photogenerated electrons and holes from inside to the surface of the material. This would result in a considerable improvement of the photocatalytic efficiency of TiO₂.

Keywords: TiO₂; Nanowire; First-principles ; Band gap; DSSCs

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