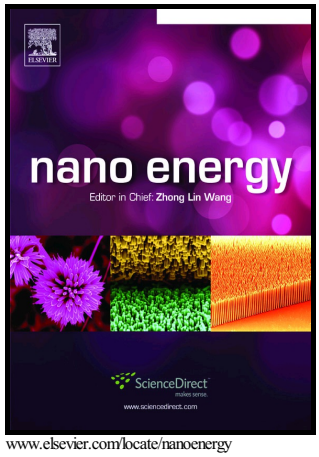

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Molecules Interface Engineering Derived External Electric Field for Effective Charge Separation in Photoelectrocatalysis

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Abstract

Realizing efficient charge separation and transfer is a key challenge for solar energy conversion. Here, we proposed the creation of an external electric field (EEF) by molecules interface engineering with silane grafting to form strong positive electricity on surface in semiconductor photocatalyst, driving charge separation and transfer in both bulk and surface. Forced by the EEF, WO_3 nanoplates anchored silane molecules (WO_3-SiH_2NH_2) for efficient photoelectrochemical (PEC) water oxidation shows 44.8% photocurrent enhancement. Interestingly, the photocurrent onset on WO_3-SiH_2NH_2 exhibited a 0.3 V negative shift from 0.5 to 0.2 V_{RHE} compared with pure WO_3 caused by the change of band edge position. The strategy of creating EEF is proven effective using other semiconductors and opens up a potential application to construct numerous high performance photoelectrodes for water splitting.

Keywords: tungsten oxide • electric field • charge separation • photoelectrocatalyst • water splitting

1. Introduction

The development of photoelectrochemical (PEC) water splitting on semiconductor electrodes is expected to become a promising route for efficient solar energy conversion.[1, 2] During the PEC process, a broad light absorption range, efficient photo-generated charge separation and fast kinetics of surface reactions with low overpotential form an excellent PEC water splitting system.[3] However, one of the major challenges causing low photoconversion efficiency is due to the fast electron-hole recombination in the semiconductor photoelectrodes. Thus, various strategies have been developed to reduce the electrons-holes recombination such as electric field construction, defect engineering, morphology and grain control, as well as loading co-catalysts.[4-10] In particular, electric field construction is mainly achieved by building p-n junction, phase junction and space charge region.[11-15] Li's group has demonstrated that an efficient charge separation across the phase junction can act as a driving force for fast charge transfer.[16] Abdi and co-workers have created a distributed homojunction by a gradient doping process, which significantly enhances the charge separation efficiency.[14] Nevertheless, most of the studies are focused on the stable separation of photoelectrons and holes on the surface of photocatalysts; whilst the minimization in the bulk charge recombination is rarely reported. The reason is that most of the photo-generated charges prefer to recombine in the bulk of photocatalyst before reaching the surface owing to the intrinsic electronic and structural properties of semiconductors. Recently, Li el. at.[17] have proposed that giant enhancement of bulk charge separation with an efficiency of 80% has been accomplished originating from 126-fold increase of internal electric field (IEF) through introducing carbon into the Bi_3O_4Cl lattice to polarize the nonuniform charge distribution. They demonstrated the significance of charge distribution caused