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## Near-complete charge separation in tailored BiVO<sub>4</sub>-based heterostructure photoanodes toward artificial leaf

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#### ABSTRACT

As an artificial leaf, a tandem device for zero-bias solar water splitting is a capable solution for practical hydrogen production. Despite a promise, poor charge transport of BiVO $_4$  hampers photoelectrochemical performances under front-side illumination, which is a hindrance to the tandem system. Herein, we design a new photoanode comprising nanoporous BiVO $_4$  and SnO $_2$  nanorods focused on the charge separation via structural and interfacial engineering. BiVO $_4$ /SnO $_2$  photoanode exhibits not only remarkable charge separation efficiency of 97% but also, by loading NiFe as a co-catalyst for water oxidation, high photocurrent density of 5.61 mA cm $^{-2}$  at 1.23 V versus the reversible hydrogen electrode under front-side 1 sun illumination. Consequently, a tandem cell comprising NiFe/BiVO $_4$ /SnO $_2$  photoanode and perovskite/Si tandem solar cell generates an operating photocurrent density of 5.90 mA cm $^{-2}$  with a solar-to-hydrogen conversion efficiency of 7.3% in zero-bias. This work would be a significant step to develop spontaneous solar hydrogen production.

### 1. Introduction

Photoelectrochemical (PEC) water splitting, which directly converts sunlight into hydrogen fuel, is one of the most sustainable solutions to stockpile solar energy. However, low solar-to-hydrogen (STH) conversion efficiency compared to its potential, has been a barrier to the commercialization, unlike a highly efficient photovoltaic (PV) system. The photovoltage generated by a single photoanode is insufficient to reach a required voltage (1.23 V + overpotential) for the water splitting reaction, resulting in a nonspontaneous reaction requiring external bias [1,2]. In this single absorber system, a trade-off between photovoltage generation and light absorption according to the bandgap limits improving PEC performances [3,4]. Thus, a tandem system consisting of dual absorbers with an optimal bandgap combination has been widely studied to maximize light harvesting by separating each absorption wavelength range [5-10]. A PEC-PV tandem system, especially, is favorable for spontaneous PEC water splitting in zero-bias due to the high STH conversion efficiency in terms of photovoltage production [2]. In this system, high photocurrent density in water oxidation of front photoanode is key to maximize the efficiency of the entire cell.

BiVO<sub>4</sub>, which is one of the most promising photoanode materials, has a suitable band gap and band edge position for water oxidation, delivering a high theoretical photocurrent density of 7.5 mA cm<sup>-2</sup> and STH conversion efficiency of 9.2% [11-13]. These PEC characteristics, however, markedly diminish under front-side illumination, and this issue hinders the implementation of PEC-PV tandem cell that requires high front PEC performance. Such a drawback is caused by the slow electron transport limiting the photocurrent generation of BiVO<sub>4</sub> [14, 15]. Namely, the short carrier diffusion length (~70 nm) of BiVO<sub>4</sub> inhibits charge separation [16]. To enhance the charge separation efficiency of BiVO<sub>4</sub>, two representative strategies are used; the first one is the nanostructuring of BiVO<sub>4</sub> [11,17,18]. Kim et al. fabricated a nanoporous BiVO<sub>4</sub> photoanode with charge separation efficiency of 90% [19], and Kuang et al. found an optimal average diameter (≈120 nm) of BiVO<sub>4</sub> to maximize PEC properties under front-side illumination [15]. The distance between the electrode inside and the electrolyte interface was structurally engineered as much the carrier diffusion length to make efficient charge transport without a reduction of light absorption. The

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