Electronic Supplementary Information

Synthesis and Characterization of Nanoporous Bi_3NbO_7 Films: Application to Photoelectrochemical Water Splitting

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Optical characteristics

UV-vis absorption spectra in the wavelength region 300-800nm of Bi_3NbO_7 films are shown in the Fig.S1. Fig. S1(a) shows the spectra of Bi_3NbO_7 films deposited at 350℃, 375℃, 400℃, 425℃, 450℃ and then annealed at 500℃ for 2h. The band gap edges are determined to be distributed from 425 nm to 450 nm with increased deposition temperatures, from which the band gap energies of Bi_3NbO_7 films distributed from 2.91eV to 2.75eV were calculated. Some researchers have reported that the optical absorption edges of Bi_3NbO_7 powder displayed a red shift with increasing the deposition temperature, which could be assigned to the decrease of the crystal particle size.[1] Fig. S1(b) shows the UV-vis spectra of Bi_3NbO_7 films with various thicknesses. There is no obvious difference of UV-vis spectra for Bi_3NbO_7 films with various thicknesses, indicating that film thickness doesn't affect the film band gap energy.

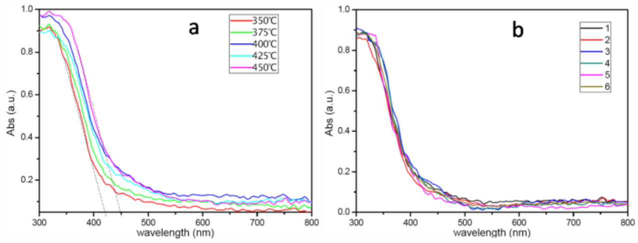

Figure S1 UV-vis absorption spectra of Bi_3NbO_7 films with (a) various deposition temperatures, (b) various thickness.

Photoelectrochemical efficiency characteristics

The solar energy to chemical energy conversion efficiency known as photo-conversion efficiency (η) of the as-prepared Bi_3NbO_7 photoanode was calculated by the following equation[2]

$$\eta(\%) = \frac{total\ power\ output - electrical\ input}{light\ power\ input}$$

$$= \frac{j_p[E_{rev}^{0} - |E_{app}|]}{I_0} \times 100 \quad (1)$$

where j_p is the photocurrent density (mA/cm^2), $j_pE^0_{rev}$ is total energy output, j_pE_{app} is the total electrical energy input and I_0 is the power density of incident light ($mW\ cm^{-2}$). E^0_{rev} refers to the standard reversible potential of 1.23 V [vs. the normal hydrogen electrode (NHE)]. The applied potential is $E_{app} = E_{means} - E_{aoc}$, where E_{means} stands for the electrode potential vs. a saturated calomel electrode (SCE) of work electrode at which the photocurrent is measured under irradiation and E_{aoc} is the electrode potential (vs. SCE) of the same work electrode under open-circuit conditions under the same irradiation and in the same electrolyte[2]. As illustrated in Fig. S2, the solar to hydrogen efficiency of Bi_3NbO_7 photoanode deposited with 3 times of repeating spray procedure at 350℃ was calculated according to equation (1). The selected sample displayed a PEC efficiency of 0.0016% at 0.7 V vs. SCE, which could be assigned to the limited optical absorption ability of Bi_3NbO_7 photoanodes that only responding to light with ultraviolet frequencies. As illustrated in the UV-vis absorption spectra (Fig. S1), the optical absorption edges of Bi_3NbO_7 were located around 400 nm, indicating restricted proportion of solar spectrum (~ 4%) could be utilized by as-prepared photoanodes. On the other hand, the fast recombination rate of the photo-induced carriers is believed another significant factor that limited the PEC performance of Bi_3NbO_7 photoanodes[3].

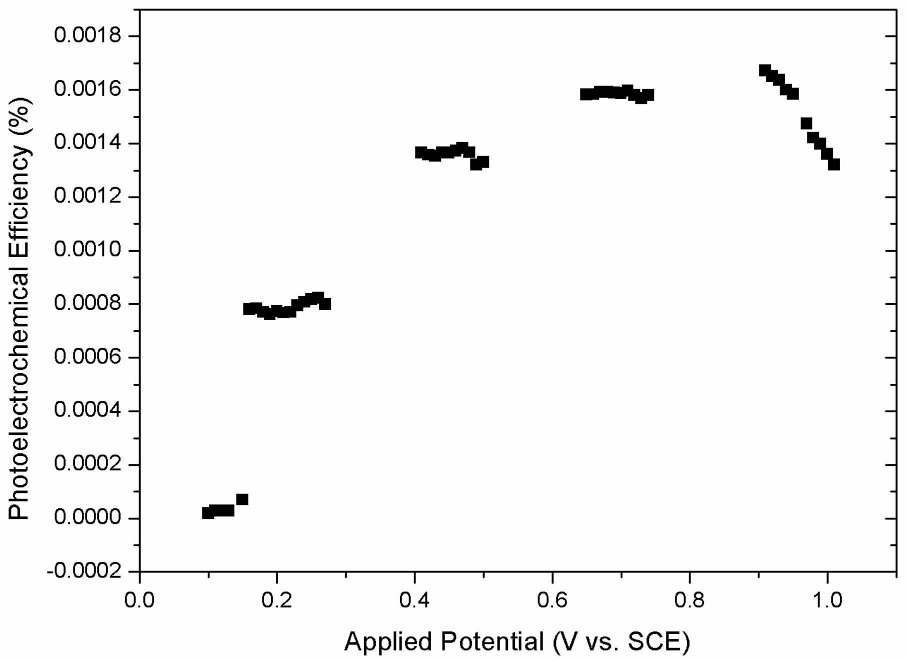

Figure S2 PEC efficiency of Bi3NbO7 photoanode deposited with 3 times of repeating spray procedure at 350℃, as a function of applied potential.

References:

1. Zhou, H.-m.; Yi, D.-q.; Yu, Z.-m.; Xiao, L.-r.; Li, J., Preparation of aluminum doped zinc oxide films and the study of their microstructure, electrical and optical properties. *Thin Solid Films* **2007,** *515* (17), 6909-6914.

2. Li, X.; Hou, Y.; Zhao, Q.; Chen, G., Synthesis and Photoinduced Charge-Transfer Properties of a ZnFe2O4-Sensitized TiO2 Nanotube Array Electrode. *Langmuir* **2011,** *27* (6), 3113-3120.

3. Hou, J.; Wang, Z.; Jiao, S.; Zhu, H., Bi2O3 quantum-dot decorated nitrogen-doped Bi3NbO7 nanosheets: in situ synthesis and enhanced visible-light photocatalytic activity. *CrystEngComm* **2012,** *14* (18), 5923-5928.