Supporting Information

Efficient charge separation and transfer of TaON/$BiVO_4$ heterojunction for photoelectrochemical water splitting

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Materials

Ta_2O_5, $Bi(NO_3)_3{\cdot}5H_2O$, $VO(acac)_2$ and p-benzoquinone were purchased from Aladdin-Reagent. All other reagents were used as purchased without further purification. The Glass slides coated with fluorine-doped tin oxide (FTO) purchased from Zhuhai Kaivo Optoelectronic Technology. FTO was cleaned by ultrasonication in ethanol, DI water and acetone before used as a substrate for the thin films.

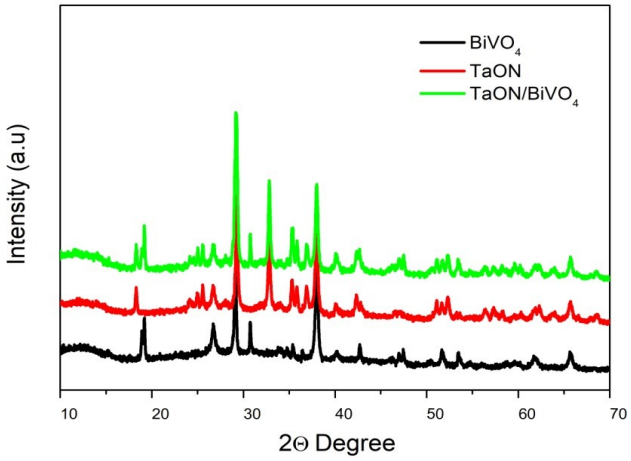

Fig. S1 XRD patterns of $BiVO_4$, the TaON and TaON/$BiVO_4$ electrodes.

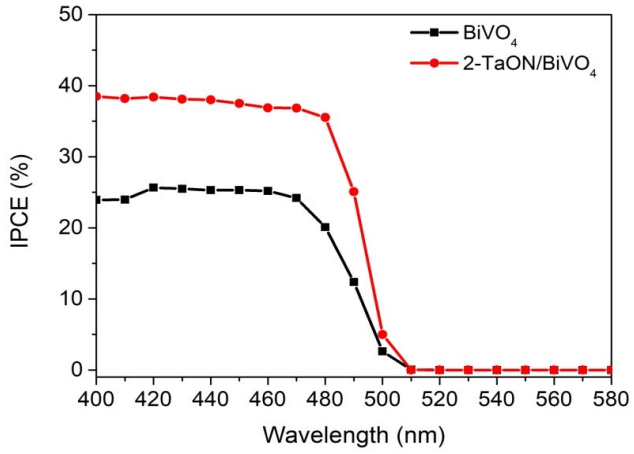

Fig. S2 The IPCE spectra of the sample electrodes.

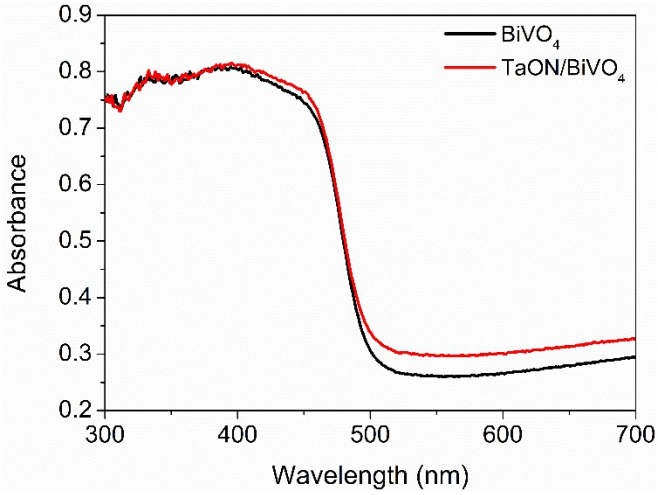

Fig. S3 UV-Vis absorption spectra of the sample electrodes.

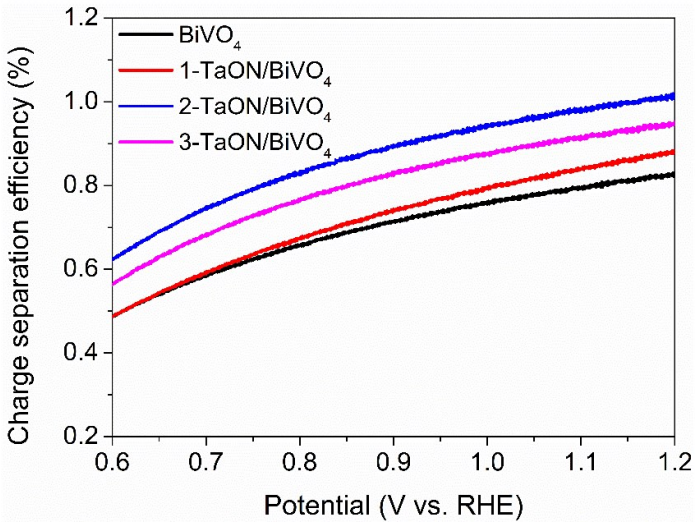

Fig. S4 The charge separation efficiency of different electrodes.

To calculate J_{abs} (the photocurrent density when the absorbed photons completely convert into photocurrent), the reference solar spectral irradiance at AM 1.5 G was converted to the solar energy spectrum in terms of number of photons vs. wavelength. Then, according to the UV-Vis absorption (Fig S3), the number of photons that $BiVO_4$ can effectively absorb was calculated using a trapezoidal integration (in 1 nm increments) of the spectrum and was converted to the current density ($mA \cdot cm^{-2}$). [1,2] Using these calculations, J_{abs} =5.6 mA/cm^2 was obtained（The effects of all electrodes calculated by this method are similar, so we uniformly take the value of 5.6 mA/cm^2）. The photocurrent density arising from PEC water oxidation can be described as: $J_{H2O} = J_{abs} \times \eta_{sep} \times \eta_{trans}$, where: η_{sep} is the charge separation efficiency, and η_{trans} is the charge injection efficiency. With Na_2SO_3 as a hole scavenger, the surface recombination is eliminated, η_{trans} = 1, and the photocurrent can be described as: $J_{Na2SO3} = J_{abs} \times \eta_{sep}$, So the η_{sep} can describe as: $\eta_{sep} = J_{Na2SO3}/J_{abs}$.

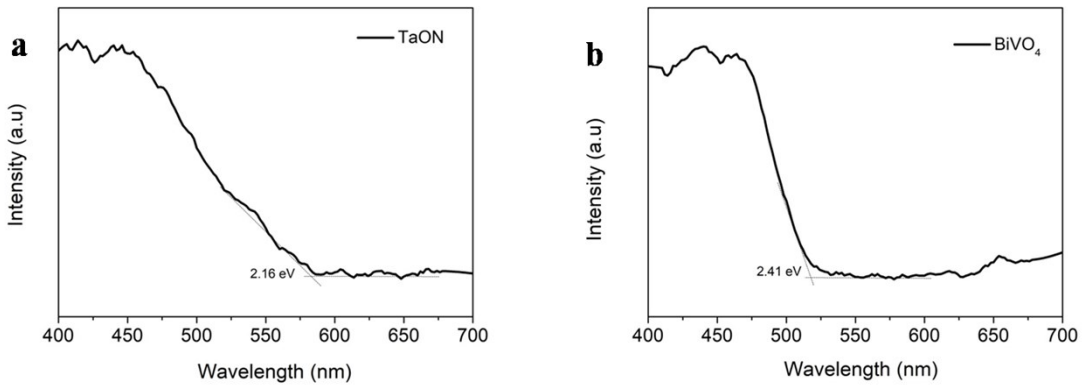

Fig. S5 UV-Vis absorption spectra of TaON and $BiVO_4$

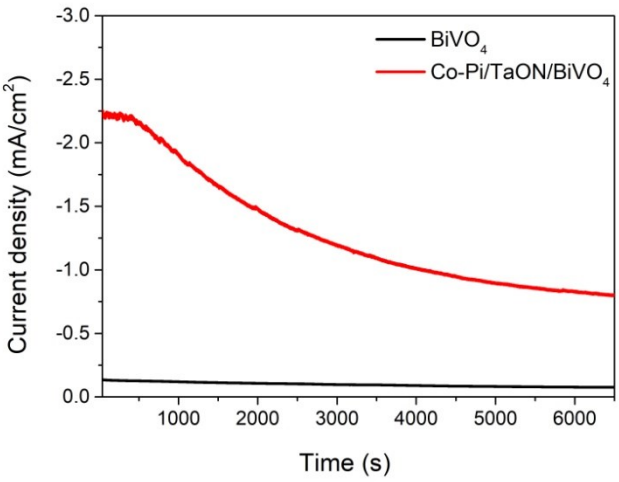

Fig. S6 I-t curves of the $BiVO_4$, Co-Pi/TaON/$BiVO_4$ electrodes at 0.8 V vs. RHE.

Table S1. The interface charge transfer resistance (R(ct)) of different electrodes.

Electrodes	$BiVO_4$	1-TaON/$BiVO_4$	2-TaON/$BiVO_4$	3-TaON/$BiVO_4$
R(ct)	329	219	203	212

[1] T. W. Kim and K.-S. Choi, Science, 2014, 343, 990-994.

[2] D. Zhou, K. Fan, Q. Zhuo, Y. Zhao, and L. Sun, ACS Appl. Mater. Interfaces, 2021, 13, 2723–2733.