Electronic Supplementary Information

Formation of Internal P–N Junctions in Ta₃N₅ Photoanodes for Water Splitting

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Electronic Supplementary Information for:

1. The influence of the Co-doping degree on the photoelectrochemical performance of the Ta₃N₅-based photoanodes.
2. The Co 2p₃/₂ XPS spectra of the Ta₃N₅:Co film.
3. The photocurrents exhibited by the bare Ta and the Ta₃N₅:Co electrodes in a polysulfide redox couple (S²⁻/S₈²⁻) solution.
4. Calculation of solar energy conversion efficiency of the Ta₃N₅:Co photoanode.
5. A stability test of the Ta₃N₅:Co electrode by conducting a long-time photoelectrochemical reaction.
1. The influence of the Co-doping degree on the photoelectrochemical performance of the Ta$_3$N$_5$-based photoanodes

Figure S1. (a) Photoresponse of the Ta$_3$N$_5$:Co photoanodes obtained at an anodic bias of 0.5 V vs. Ag/AgCl and illuminated with chopped AM 1.5G simulated sunlight at 100 mW cm$^{-2}$. The photoanodes were obtained using Co(NO$_3$)$_2$ soaking solutions of varying concentrations (0–1 M). The electrolyte is a 0.5-M KOH aqueous solution (pH=13.6). (b) Variation of the photocurrent with the concentration of the Co(NO$_3$)$_2$ soaking solution.
2. The Co 2p$_{3/2}$ XPS spectra of the Ta$_3$N$_5$:Co film

Figure S2. (a) The Co 2p$_{3/2}$ XPS spectra of the as-received Ta$_3$N$_5$:Co film. The Co ions likely belong to Co$_{5.47}$N because their binding energy is close to that of Co metal. (b) The Co 2p$_{3/2}$ XPS spectra of the Ta$_3$N$_5$:Co film after the PEC reaction. The Co ions were oxidized to high-valence Co ions, likely belonging to Co$_2$O$_3$/Co$_3$O$_4$ (i.e., CoO$_x$)$_{1,2}$
3. The photocurrents exhibited by the bare Ta and the Ta₃N₅:Co electrodes in a polysulfide redox couple (S²⁻/Sₓ²⁻) solution

![Graph showing photocurrent density vs potential for Ta₃N₅ and Ta₃N₅:Co photoanodes.]

**Figure S3.** Current-potential characteristics of the Ta₃N₅ and Ta₃N₅:Co photoanodes with an anodic scan applied at 10 mV s⁻¹ and illuminated with AM 1.5G simulated sunlight at 100 mW cm⁻². The electrolyte is a fast polysulfide redox couple (S²⁻/Sₓ²⁻) aqueous solution containing 0.24 M Na₂S and 0.35 M Na₂SO₃.
4. Calculation of solar energy conversion efficiency of the Ta$_3$N$_5$:Co photoanode

**Figure S4.** Applied bias photon-to-current conversion efficiency ($\eta$) of the Ta$_3$N$_5$:Co photoanode under varying bias potentials. The $\eta$ values were calculated using the data of Fig. 7.$^{3,4}$
5. A stability test of the Ta$_3$N$_5$:Co electrode by conducting a long-time photoelectrochemical reaction

**Figure S5.** Photoresponse of the Ta$_3$N$_5$:Co photoanode obtained at an anodic bias of 0.53 V vs. counter (or 0.39 V vs. Ag/AgCl) and illuminated with AM 1.5G simulated sunlight at 100 mW cm$^{-2}$.
References


