

Supporting Information

Cathodic shift of a photo-potential on a Ta₃N₅ photoanode by post-heating a TiO₂ passivation layer

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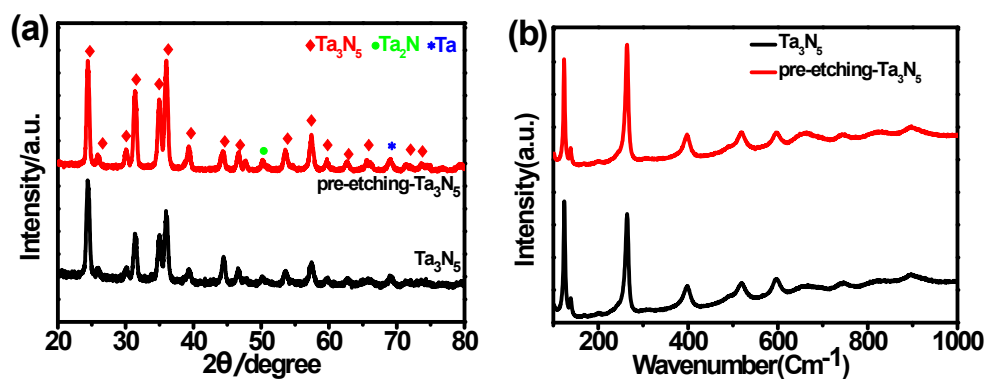


Fig. S1. (a) X-ray diffraction and (b) Raman spectra of Ta₃N₅ from Ta foil precursor without and with surface etching.

Table S1. The crystal grain size of Ta_3N_5 from Ta foil precursor without and with surface etching caculated from Figure S1by the Scherrer equation.

	crystallite size(nm)	
Peak position	Ta_3N_5	Pre-etching- Ta_3N_5
24.4	17.8	19.1
31.4	15.7	16.6
35.9	15.3	16.0

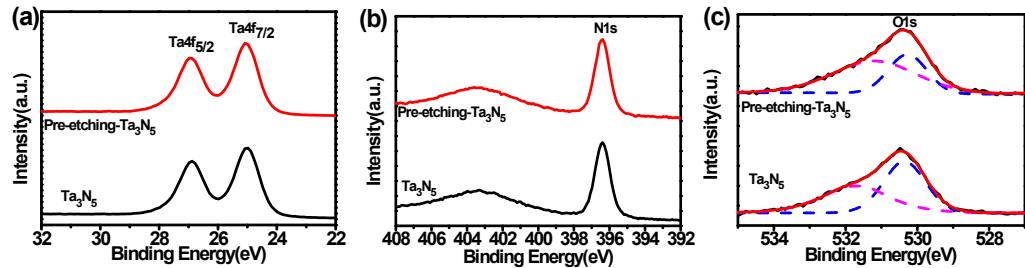


Fig. S2. XPS spectra of (a) Ta4f, (b) N1s, (c) Measured and simulated XPS spectra of O1s of as-prepared Ta_3N_5 samples from Ta foil precursor without and with surface etching.

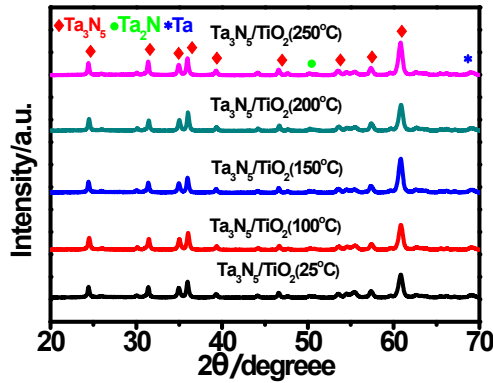


Fig. S3. X-ray diffraction patterns of $\text{Ta}_3\text{N}_5/\text{TiO}_2(25^\circ\text{C})$, $\text{Ta}_3\text{N}_5/\text{TiO}_2(100^\circ\text{C})$, $\text{Ta}_3\text{N}_5/\text{TiO}_2(150^\circ\text{C})$, $\text{Ta}_3\text{N}_5/\text{TiO}_2(200^\circ\text{C})$, $\text{Ta}_3\text{N}_5/\text{TiO}_2(250^\circ\text{C})$.

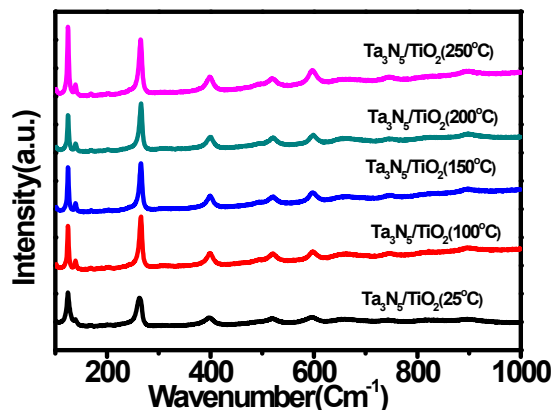


Fig. S4. Raman spectra of Ta₃N₅/TiO₂ (25°C), Ta₃N₅/TiO₂ (100°C), Ta₃N₅/TiO₂ (150°C), Ta₃N₅/TiO₂ (200°C), Ta₃N₅/TiO₂ (250°C).

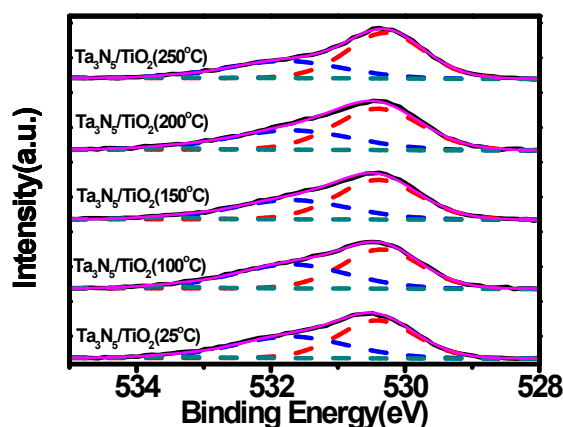


Fig. S5. Measured and simulated XPS spectra of O1s on the surface of Ta₃N₅/TiO₂ (25°C), Ta₃N₅/TiO₂ (100°C), Ta₃N₅/TiO₂ (150°C), Ta₃N₅/TiO₂ (200°C), Ta₃N₅/TiO₂ (250°C).

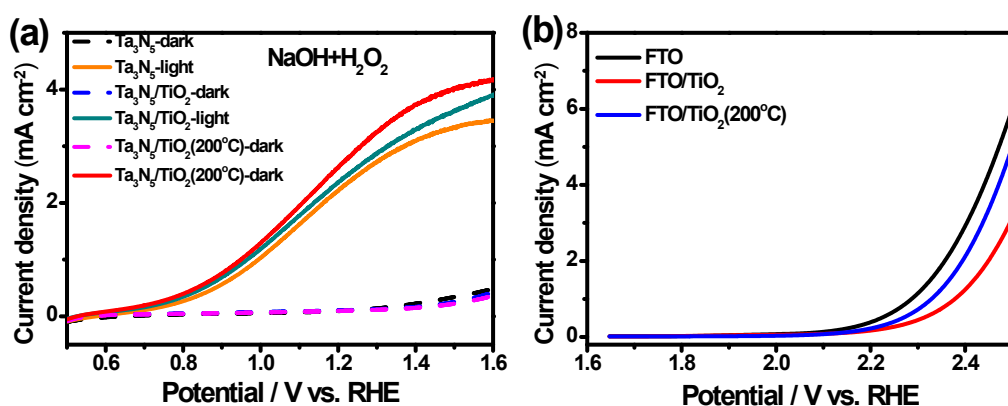


Fig. S6. (a) Current-potential curves of Ta₃N₅, Ta₃N₅/TiO₂, Ta₃N₅/TiO₂(200°C) samples with H₂O₂ as sacrificial reagent in 1M NaOH (pH=13.6) under 300W Xenon lamp irradiation; (b) Current-potential curves of FTO, FTO/TiO₂, FTO/TiO₂(200°C) samples in 1M NaOH (pH=13.6).

We measured photocurrent-potential curves of Ta₃N₅ before and after depositing TiO₂

layer in 1M NaOH (pH=13.6) with H₂O₂ as sacrificial reagent and the results are shown in Fig. S6a. Photocurrent (J_p) of a sample can be described by equation¹:

$$J_p = J_{abs} \times \eta_{sep} \times \eta_{inj}$$

Where J_p is photocurrent density (mA cm⁻²); J_{abs} is photocurrent density from absorbed light; η_{sep} is charge separation efficiency and η_{inj} is interfacial charge transfer efficiency. J_{abs} of a Ta₃N₅ photoelectrode is close to that a Ta₃N₅ photoelectrode with a TiO₂ layer because TiO₂ is too thin to absorb the light. When H₂O₂ is used as sacrificial reagent, η_{inj} is about 100%. Therefore, the photocurrent of Ta₃N₅ (J_p) in the solution with sacrificial reagent is only determined by charge separation efficiency (η_{sep}).

Reference:

1. Z. Li, W. Luo, M. Zhang, J. Feng and Z. Zou, *Energy Environ. Sci.*, 2013, **6**, 347-370.