Supporting Information

Modification of 1D TiO_2 nanowires with GaO_xN_y by atomic layer deposition for TiO_2@GaO_xN_y core-shell nanowires with enhanced photoelectrochemical performance

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Supplementary Figures

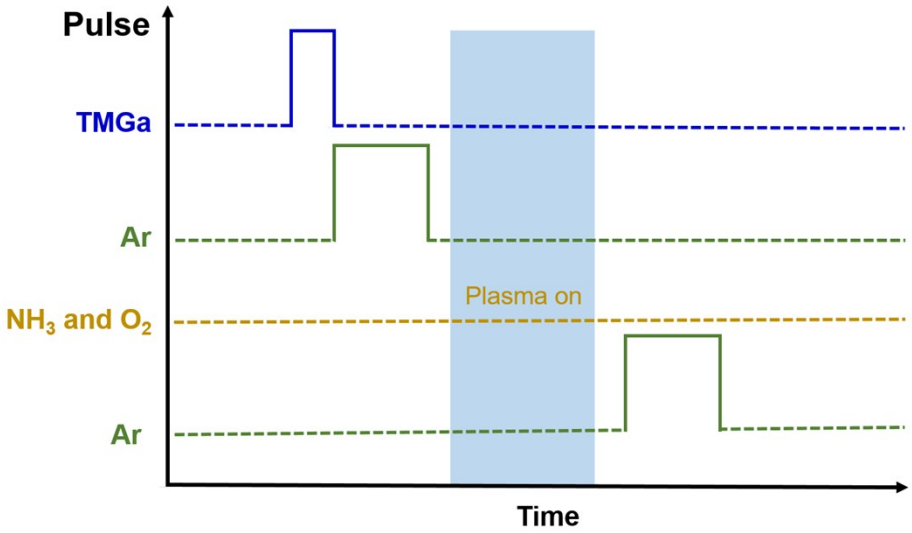

Fig. S1 The schematic diagram of one ALD cycle of GaO_xN_y deposition.

A schematic diagram of one ALD cycle of GaO_xN_y deposition is shown in Fig. S1. Typically, one ALD cycle has four steps: pulse 1 - purge 1 - pulse 2 - purge 2. Accordingly, one ALD cycle for GaO_xN_y can be described as follows: TMGa pulse (15 ms) - Ar purge (10 s) - plasma processing (15 s) - Ar purge (10 s).

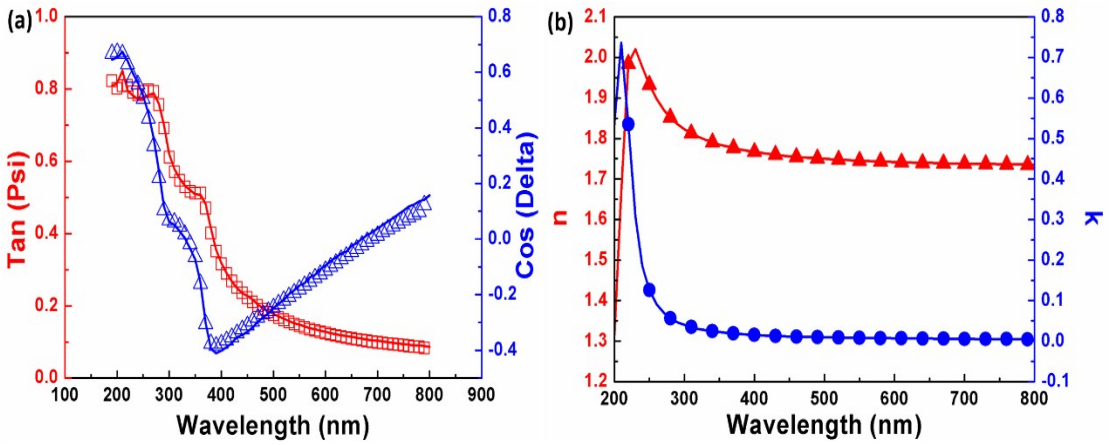

Fig. S2 (a) Measured (symbol) and fitted (line) ellipsometric data and (b) optical constants of GaO_xN_y thin films with 200 ALD cycles deposited on a Si substrate.

The fitting results show a good agreement with the experimental data in the entire measured wavelength range with RMSE≈0.99. From the SE results, it can be concluded that the thickness is 9.12 nm, the refractive index value (n) is 1.740, and the extinction coefficient (k) is 6.51×10^{-3} at a wavelength of 632.8 nm for 200 ALD cycles of GaO_xN_y samples. The obtained film thickness is nearly unchanged and agrees well the measured SEM results (Manuscript), implying the accuracy and reliability of the ellipsometric fitting. The refractive index value n and extinction coefficient k decreases with the wavelength increase in the long range, which can be seen that our results agree well with the literature for PEALD growth of AZO thin films[1].

Notes and references

1. T. Gu, E.T. Hu, S. Guo, Y. Wu, J. Wang, Z.Y. Wang, K.H. Yu, W. Wei, Y.X. Zheng, S.Y. Wang and L.Y. Chen, *Vacuum*, 2019, **163**,69-74.

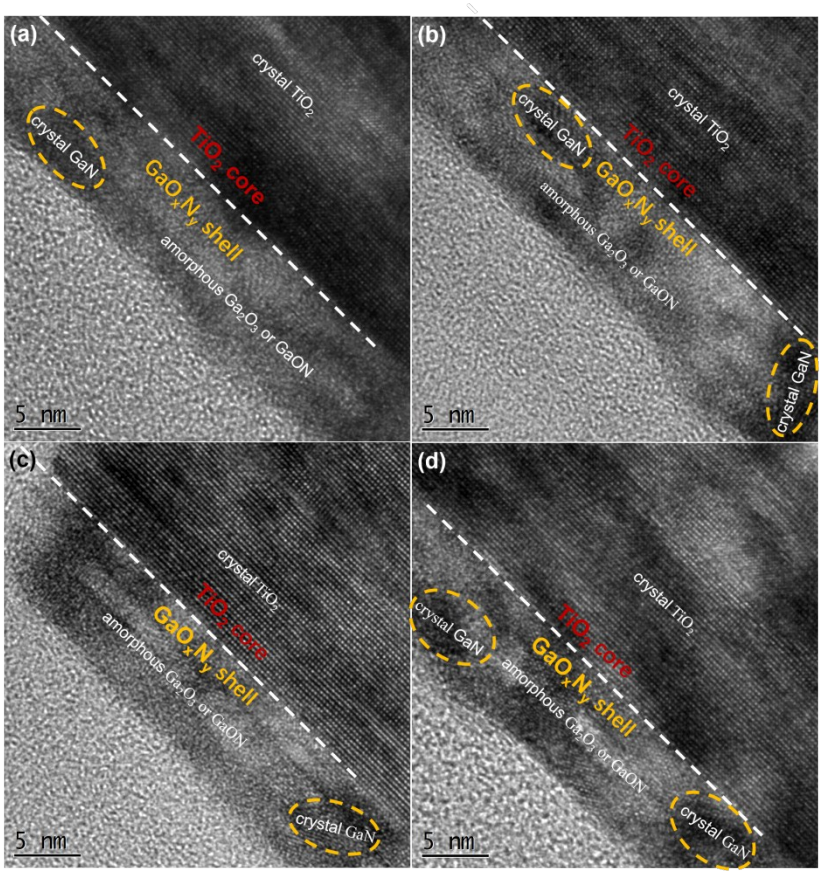

Fig. S3 HRTEM image of TG10 with different area.

The HRTEM image of the TG10 as shown in Fig. S3 indicates a poor crystallinity of GaO_xN_y shell. This is used to prove that the content of GaN crystal in GaO_xN_y is very small, and most of them are amorphous Ga_2O_3 and GaON.

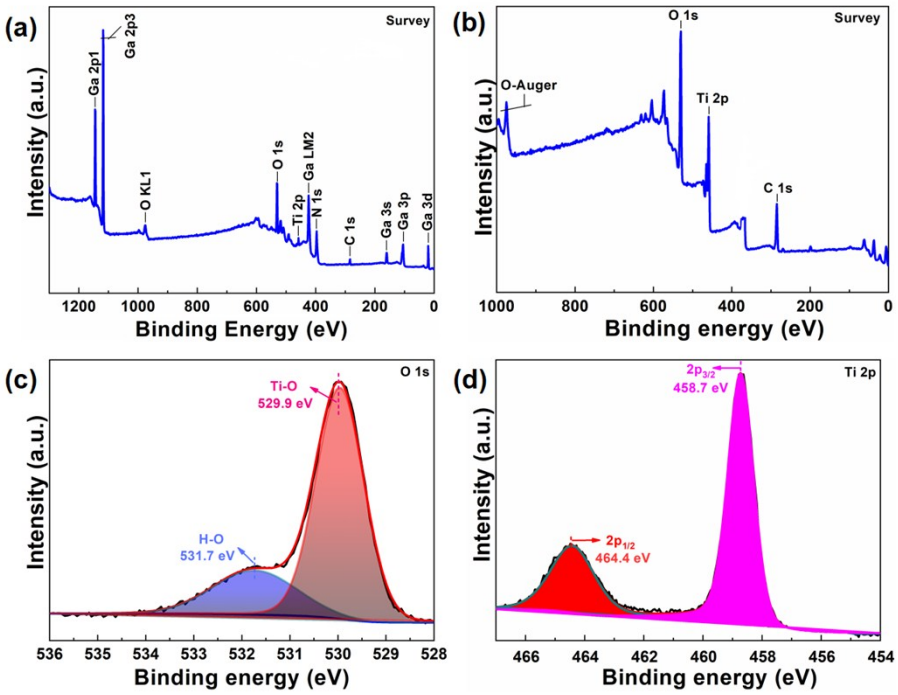

Fig. S4 XPS survey spectrum of (a) TG5, (b) TiO_2, and (c) high-resolution curve of O 1s, (d) high-resolution curve of Ti 2p.

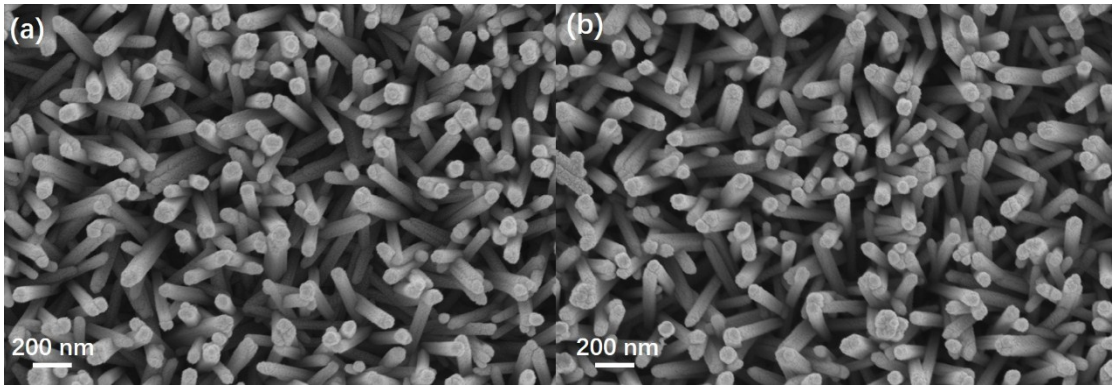

Fig. S5 The SEM image of TG20 (a) before and (b) after PEC measurements.

The SEM images of TG20 before and after PEC measurement in Fig.S5 shows no noticeable degradation of the TG20 NWs. The results also reveal that TG20 has excellent structural stability and photoelectric durability for PEC water splitting.

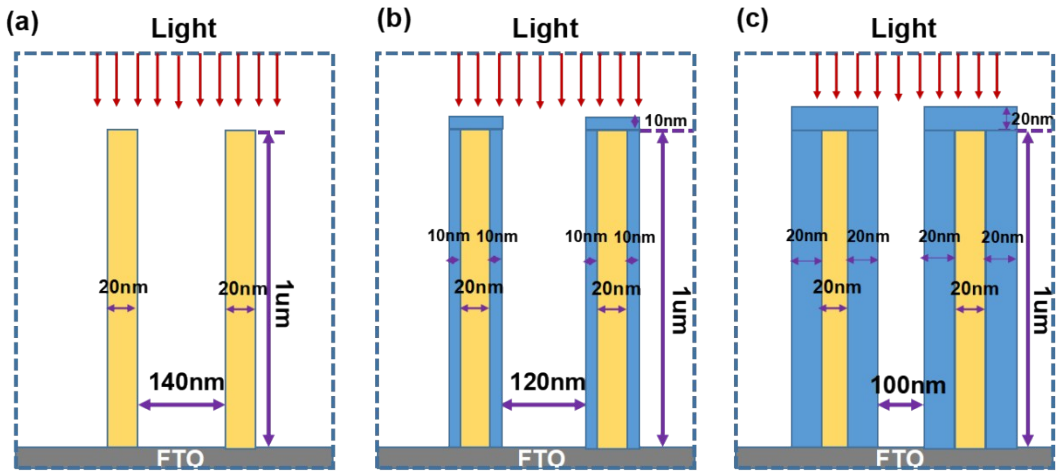

Fig.S6 Schematics of the FDTD simulation models of (a) TiO_2, (b) TG10, and (c) TG20, respectively.

The simulation models of TiO_2 and TG NWs structure are illustrated in Fig. S6. It contains TiO_2 NWs with length and width of 1 μm and 20 nm, and GaO_xN_y film with thickness of 10 and 20 nm.

Supplementary Tables

Table S1 Parameters deduced from photoelectrochemical studies for the TiO_2 and TG NWs.

Samples	**Sample details**	**R_{ct} (Ω cm^{-2})**	**Photocurrent density (mA cm^{-2}) at 1.23 V vs RHE**	**IPCE(%) at 380 nm**
TiO_2 NWs	TiO_2 Nanowires	34.56	0.08	30.44
TG5	5 nm-GaON/ TiO_2 Nanowires	30.05	0.17	-
TG10	10 nm-GaON/ TiO_2 Nanowires	26.28	0.36	-
TG15	15 nm-GaON/ TiO_2 Nanowires	23.54	0.63	-
TG20	**20 nm-GaON/ TiO_2 Nanowires**	**21.20**	**1.10**	**92.08**
TG25	25 nm-GaON/ TiO_2 Nanowires	20.32	1.02	-