

Borocarbonitride Layers on Titanium Dioxide Nanoribbons for Efficient Photoelectrocatalytic Water Splitting

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Materials and Methods

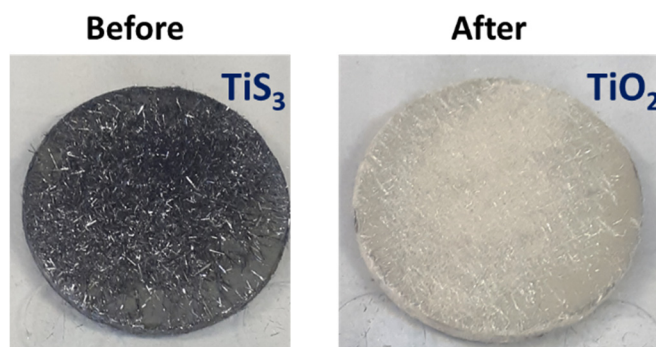


Figure S1. Photograph of a sample before and after the oxidation.

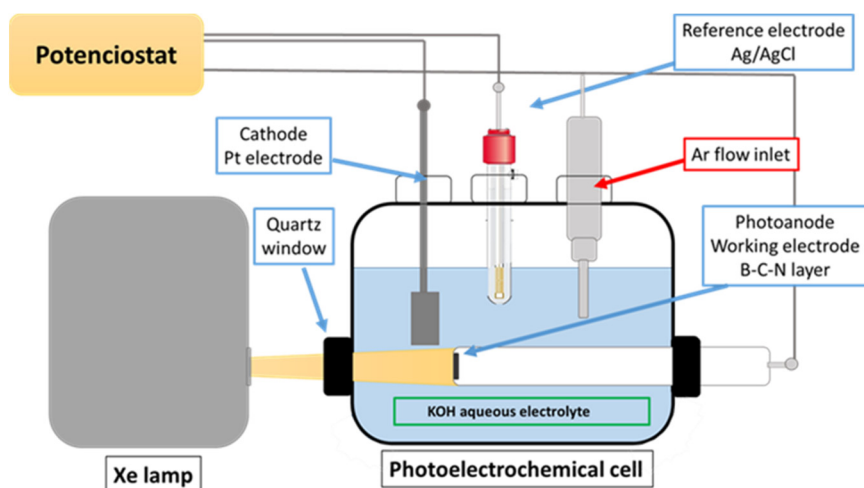


Figure S2. Scheme of the photoelectrochemical cell used in this work.

Results and Discussion

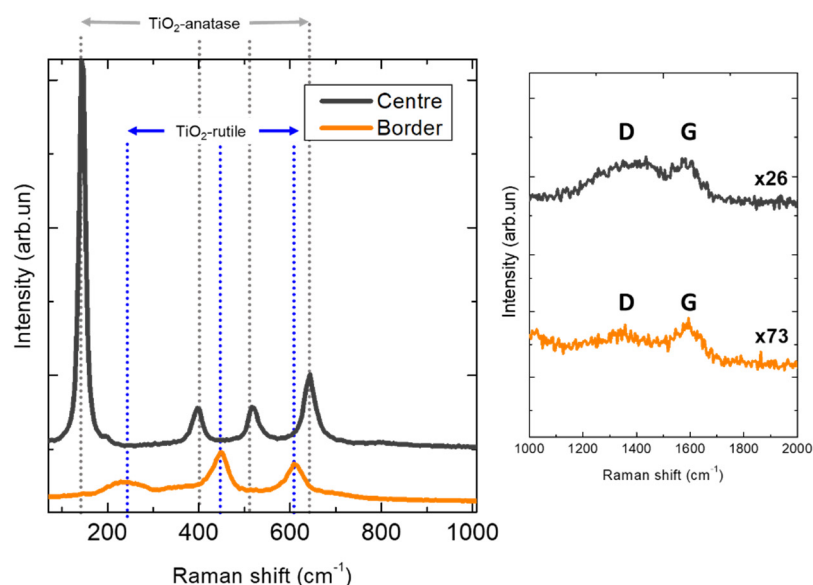


Figure S3. Raman spectra of one of the samples with BCN. The spectra has been measured in an external nanoribbon (border) and one in the center of the sample.

Table S1. Position (binding energy, BE), full peak width at a half maximum (FWHM) , and relative intensities (with and without oxygen contribution) for the TiO2-BCN and bare TiO2 samples.

Sample	Core level	Core level component	BE (eV)	FWH M (eV)	Area	Relative intensity (%)	Relative intensity excluding oxygen (%)
TiO2-BCN	B1s	B-C	189.40	1.21	87.52	12.39	3.85
		B-N	190.87	1.95	156.62	22.17	64.15
		B-O	192.70	2.45	462.40	65.45	
	C1s	C-B	282.91	1.20	25.12	2.29	2.53
		C-C	284.64	1.73	849.17	77.48	85.47
		C-N	285.48	1.56	120.37	10.98	12.10
		C-Ox	286.43	1.52	101.29	9.24	
	Ti2p	Ti3+ (Ti2p _{3/2})	457.55	0.61	9.04	0.45	
		Ti4+ (Ti2p _{3/2})	459.50	1.47	1207.50	60.77	
		Ti4+ (Ti2p _{1/2})	465.15	2.47	770.31	38.77	
TiO2	Ti2p	Ti4+ (Ti2p _{3/2})	459.60	1.39	5378.50	62.31	
		Ti4+ (Ti2p _{1/2})	465.29	2.35	3253.50	37.69	

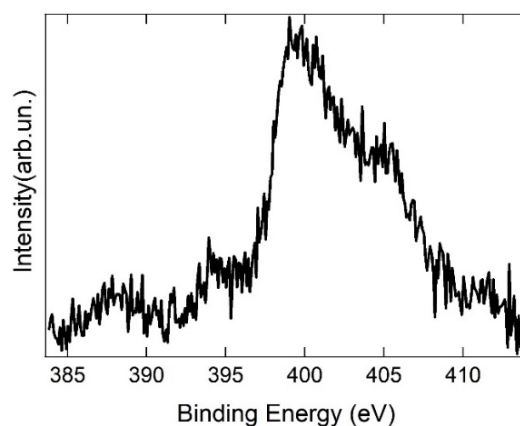


Figure S4. XPS measurement between 384eV and 413 eV. N1s is overlapped with a small signal of the Ta4p_{3/2} peak, ascribed to the tantalum clips used to fix the sample to the sample holder.

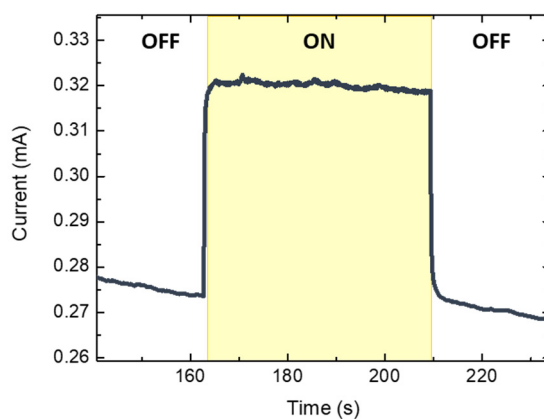


Figure S5. Photocurrent of TiO₂-BCN heterostructure under Xe lamp illumination at 0.6 V vs Ag/AgCl in 0.1 M KOH aqueous solution.

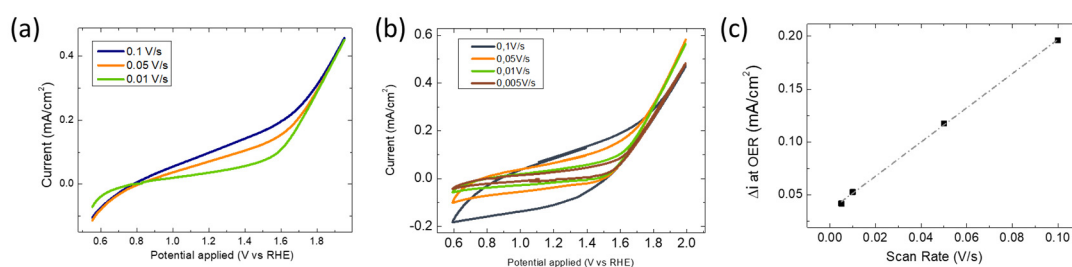


Figure S6. (a) LSW at different scan rates (b) CV at different scan rates (c) Difference between the anodic and cathodic current of the CV measurements.

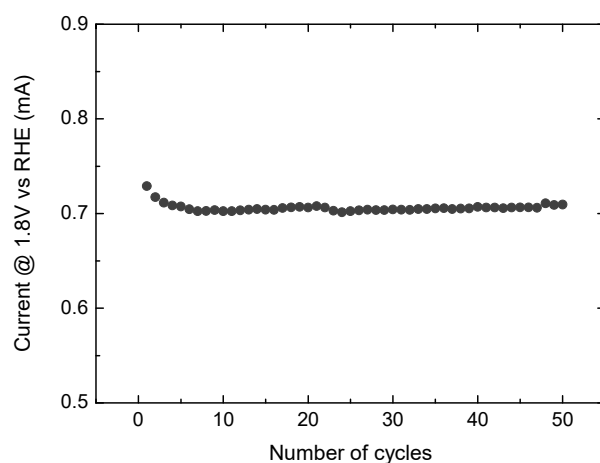


Figure S7. To prove the stability of our electrode, series of cyclic voltammetry at 0.05mV/s have been done. This figure shows the current at the maximum potential applied (1.8V vs RHE) for each one of the cycles, for the TiO₂-BCN sample in 1.0M KOH aqueous electrolyte.

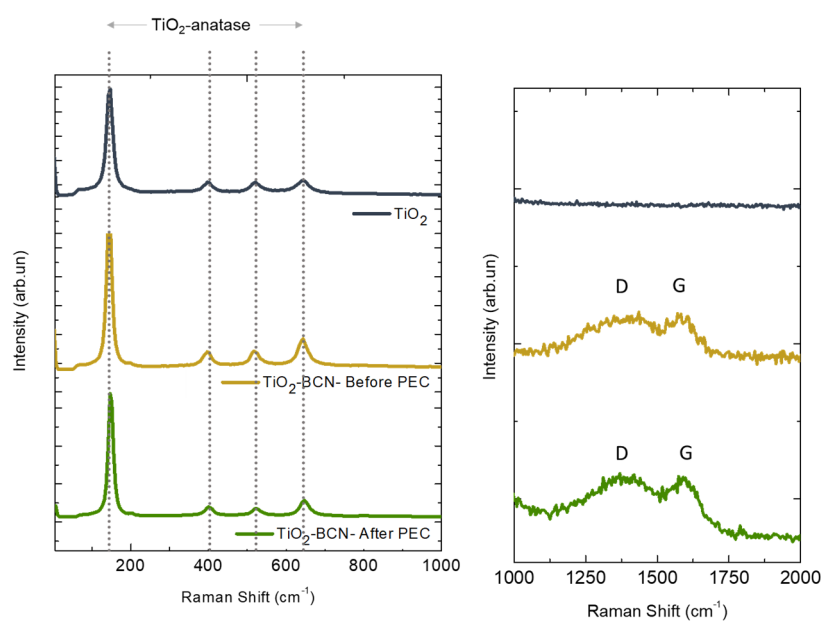


Figure S8. Raman spectra of TiO₂ and TiO₂-BCN before the photoelectrochemical measurements (PEC) and TiO₂-BCN after the PEC.

Table S2. Comparison between TiO₂ and TiO₂-BCN of the current density in dark condition at 1.85V vs RHE (I_{dark}), photocurrent at 1.85V vs RHE (I_{ph}) and flat band potential.

	TiO ₂	TiO ₂ -BCN
I_{dark} (@ 1.85V vs RHE)	0.006 $\mu\text{A}/\text{cm}^2$	0.071 $\mu\text{A}/\text{cm}^2$
I_{ph} (@ 1.85V vs RHE)	1.78 μA	47.6 μA
E_{fb}	0.2 ± 0.1 V vs RHE	0.2 ± 0.1 V vs RHE

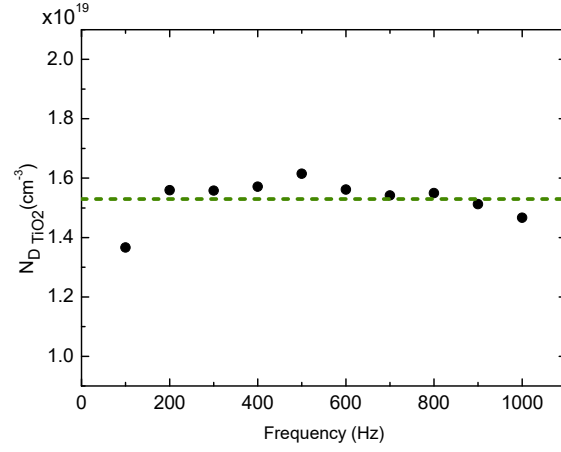


Figure S9. Donor density of the TiO₂ sample.

Table S3. Fitting parameters of graphs Figure 7c and d, to an exponential decay: $y = y_0 + A \cdot \exp\left(-\frac{f}{t}\right)$ where y is the parameter of the Y-axis, and f is the frequency.

	y_0	A	t
$\frac{\epsilon_{\text{TiO}_2\text{-BCN}} \cdot N_{D\text{TiO}_2\text{-BCN}}}{\epsilon_{\text{TiO}_2} \cdot N_{D\text{TiO}_2}}$	7.6 ± 0.6	133 ± 2	236 ± 6
$\epsilon_{\text{TiO}_2\text{-BCN}} \cdot N_{D\text{TiO}_2\text{-BCN}}$	$(3.0 \pm 0.5) \cdot 10^{22}$	$(9.3 \pm 0.4) \cdot 10^{23}$	$(1.5 \pm 0.2) \cdot 10^2$