Electronic Supplementary Material (ESI) for RSC Sustainability.

Supplementary Information

Dual heterojunctions-based Au@TiO_2 photoelectrode exhibiting efficient charge separation for enhanced removal of organic dye under visible light

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Table S1 Parameters of photoelectrochemical measurements of A-FH TiO_2/Ti, 1%Au@A-FH TiO_2/Ti, 2%Au@A-FH TiO_2/Ti and 4%Au@A-FH TiO_2/Ti.

Photoelectrode	Photocurrent (10^{-5}A cm^{-2})	Resistance value (10^3 Ω)	Donor density (N_D:×10^{20} cm^{-3})
A-FH TiO_2/Ti	0.70	14	1.27
1%Au@A-FH TiO_2/Ti	0.75	12	1.58
2%Au@A-FH TiO_2/Ti	1.15	5	2.67
4%Au@A-FH TiO_2/Ti	0.90	7.5	2.43

Table S2 The bend enrgy (BE) position and raw area of A-FH TiO_2/Ti and Au@A-FH TiO_2/Ti.

Photoelectrode	Peak	Split Peak	Position BE (eV)	Raw Area (cps eV)
A-FH TiO_2/Ti	Ti 2p	Ti^{4+} $2p_{3/2}$	**458.7**	**10837.9**
		Ti^{4+} $2p_{1/2}$	**464.4**	
	O 1s	Ti-O-Ti	**529.9**	**19262.1**
		Ti-O-H	**532.7**	
Au@A-FH TiO_2/Ti	Ti 2p	Ti^{4+} $2p_{3/2}$	**458.9**	**7241.4**
		Ti^{4+} $2p_{1/2}$	**464.6**	
	O 1s	Ti-O-Ti	**530.2**	**10957.2**
		Ti-O-H	**533.0**	
	Au 4f	Au^0 $4f_{7/2}$	**83.0**	**3173.9**
		Au^0 $4f_{5/2}$	**86.8**	

Table S3 The light absorption (η_{abs}), charge separation (η_{sep}), and injection efficiency (η_{inj}) of all photoelectrodes.

Photoelectrode	η_{abs}	η_{sep}	η_{inj}
Au@A-TiO_2/Ti	**32.6 %**	**1.1 %**	**7.9 %**
A-FH TiO_2/Ti	**45.2 %**	**1.3 %**	**20.2 %**
Au@A-FH TiO_2/Ti	**54.5 %**	**3.9 %**	**40.8 %**

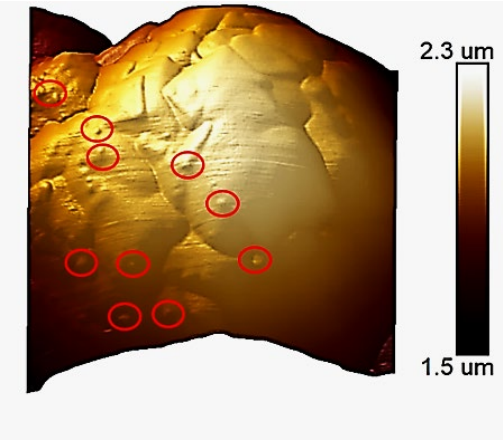

Fig. S1 AFM 3D diagram of Au@A-FH TiO_2/Ti.

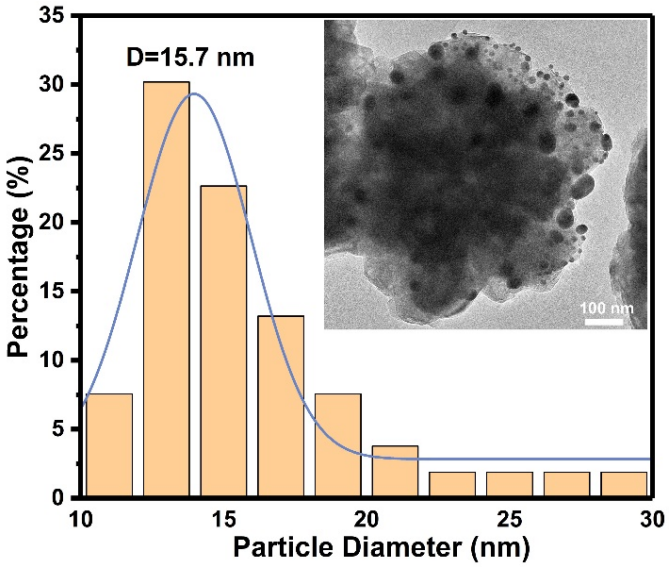

Fig. S2 Au particle size distribution of 2%Au@A-FH TiO_2/Ti.

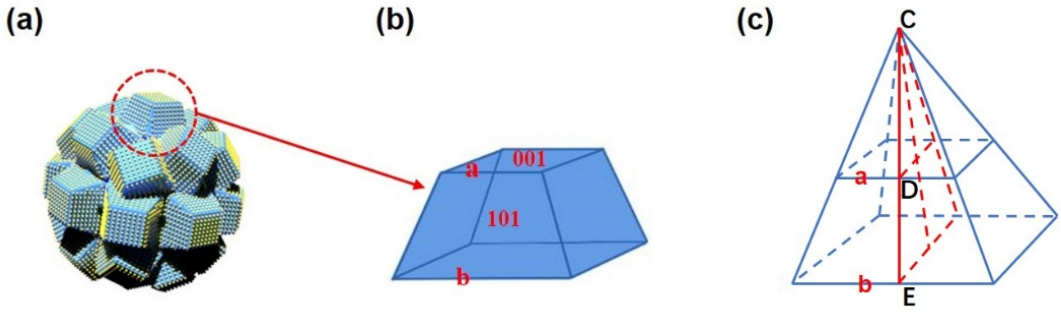

Fig. S3 Model schematic of (a) nanoflower-like TiO_2 microspheres, (b) truncated tetragonal pyramid and (c) truncated pyramid.

The exposure percentage of {001} facet is about 70% calculated by the formula below:

$$S_{\{001\}\exp}(\%) = S_{\{001\}} / (S_{\{101\}} + S_{\{001\}})$$
$$= 2a^2 / [2a^2 + 8\times(0.5\ \mathrm{CE}\times b - 0.5\ \mathrm{CD}\times a)]$$
$$= cos\theta / [cos\theta + (a/b)^{-2} - 1]$$

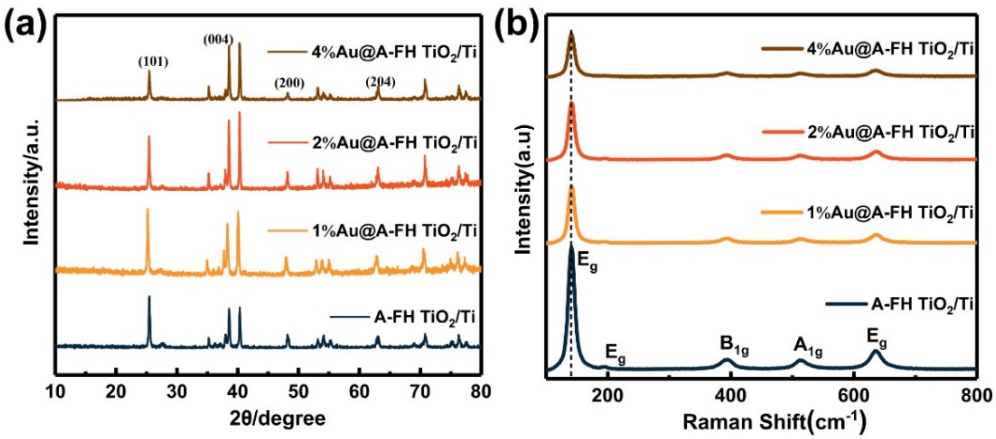

Fig. S4 The XRD patterns (a) and Raman spectra (b) of photoelectrodes.

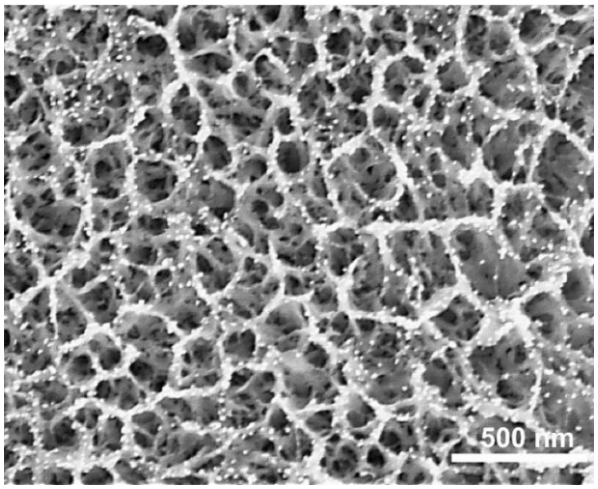

Fig. S5 SEM images of Au@A-TiO_2/Ti without specific crystal facet.

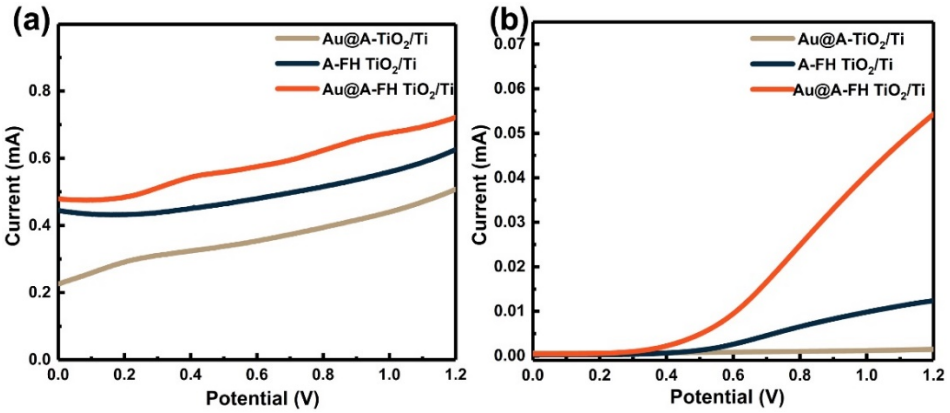

Fig. S6 LSV curves in 0.1 M Na_2SO_4 (a) and Na_2SO_3 (b) solution of three samples under AM1.5G illumination.

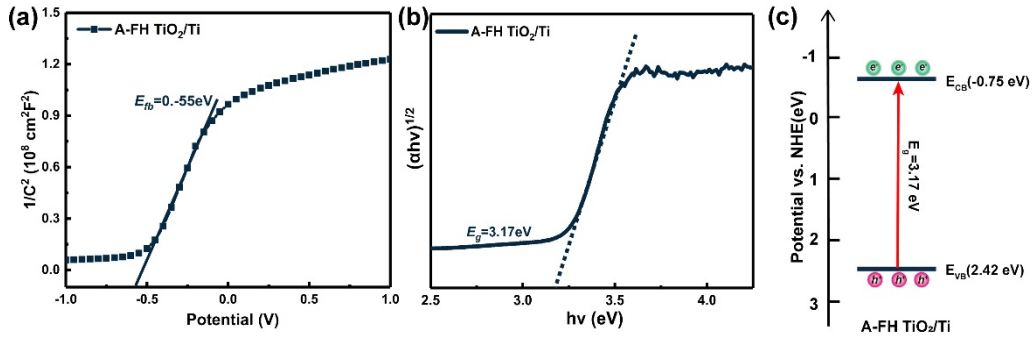

Fig. S7 The band structure diagram (c) calculated by band gap value (a) and flat band (b) of A-FH TiO2/Ti.

The conduction band (E_{CB}) of TiO_2 is generally considered to be more negative by 0.2 eV relative to the flat band (E_{fb}).

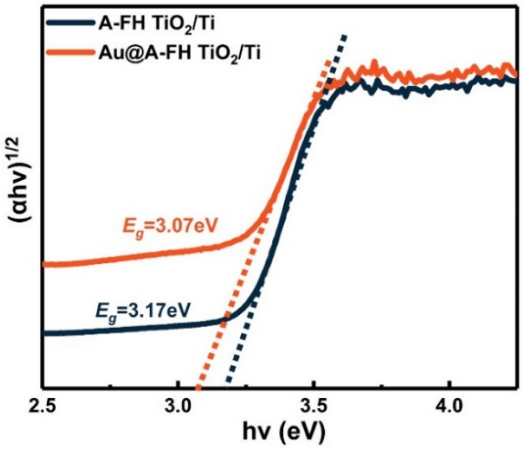

Fig. S8 Calculated band gap energy of A-FH TiO_2/Ti and Au@A-FH TiO_2/Ti.

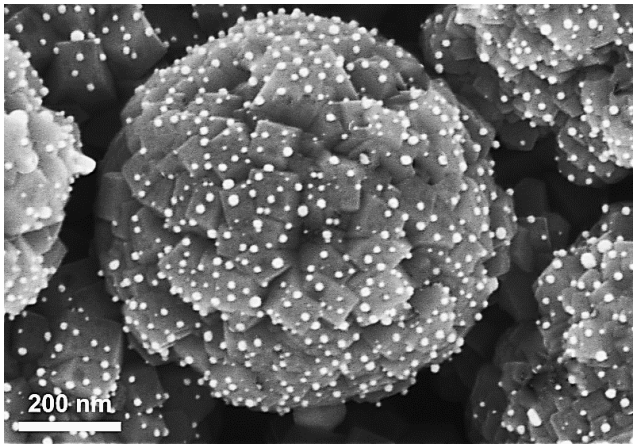

Fig. S9 The SEM images of Au@A-FH TiO_2/Ti after 5 cycles.

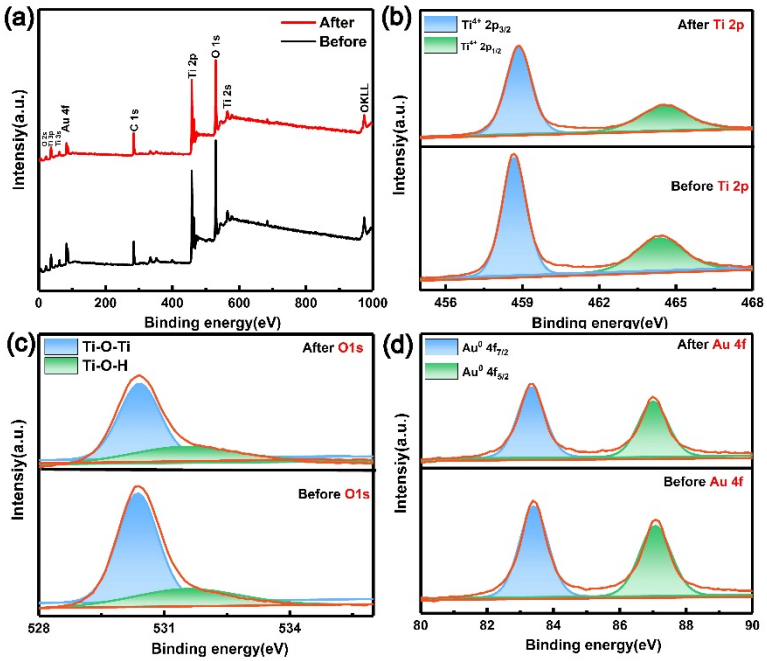

Fig. S10 The XPS spectra (a), Ti 2p (b), O 1s (c) and Au 4f (d) spectra of A-FH TiO_2/Ti and Au@ A-FH TiO_2/Ti after five cycles.

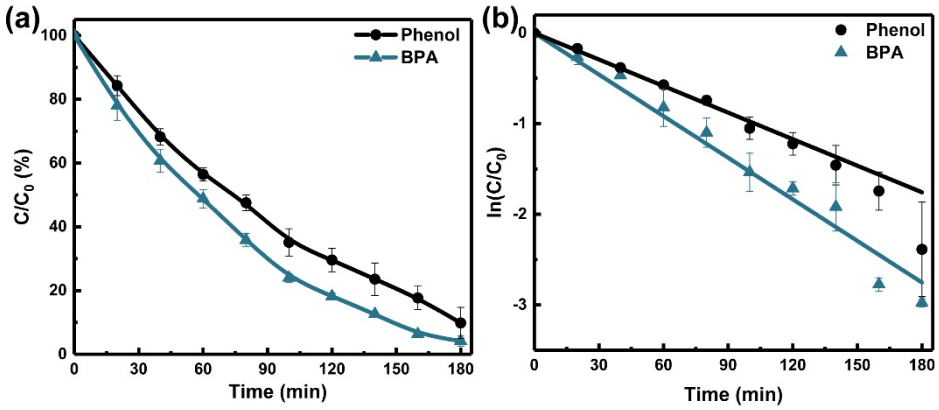

Fig. S11 The degradation and first order kinetic curves for phenol and Bisphenol A degradation