Electronic Supplementary Material (ESI) for Nanoscale Advances.

Visible Light Active Zr and N Doped TiO_2 Coupled g-C_3N_4 Heterojunctions Nanosheet as Photocatalysts for Degradation of Bromoxynil and Rh B along with H_2 Evolution Process

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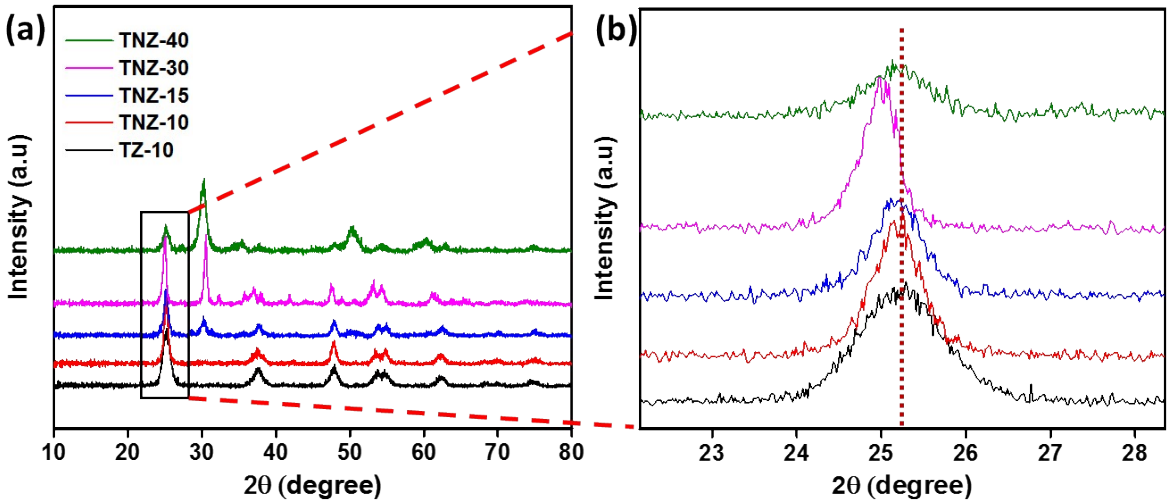


Figure S1 (a) XRD plot of Zr and N doped titania with a varying dopant concentration of Zr from 10-40 wt% and also N undoped TZ-10 system. **(b)** represents the enlarged picture of the (101) plane shifting to the lower diffraction angle.

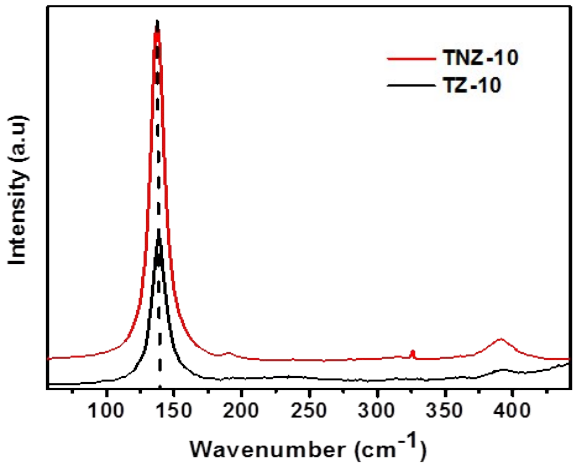


Figure S2. Raman spectra of N doped TNZ -10 and undoped TZ -10

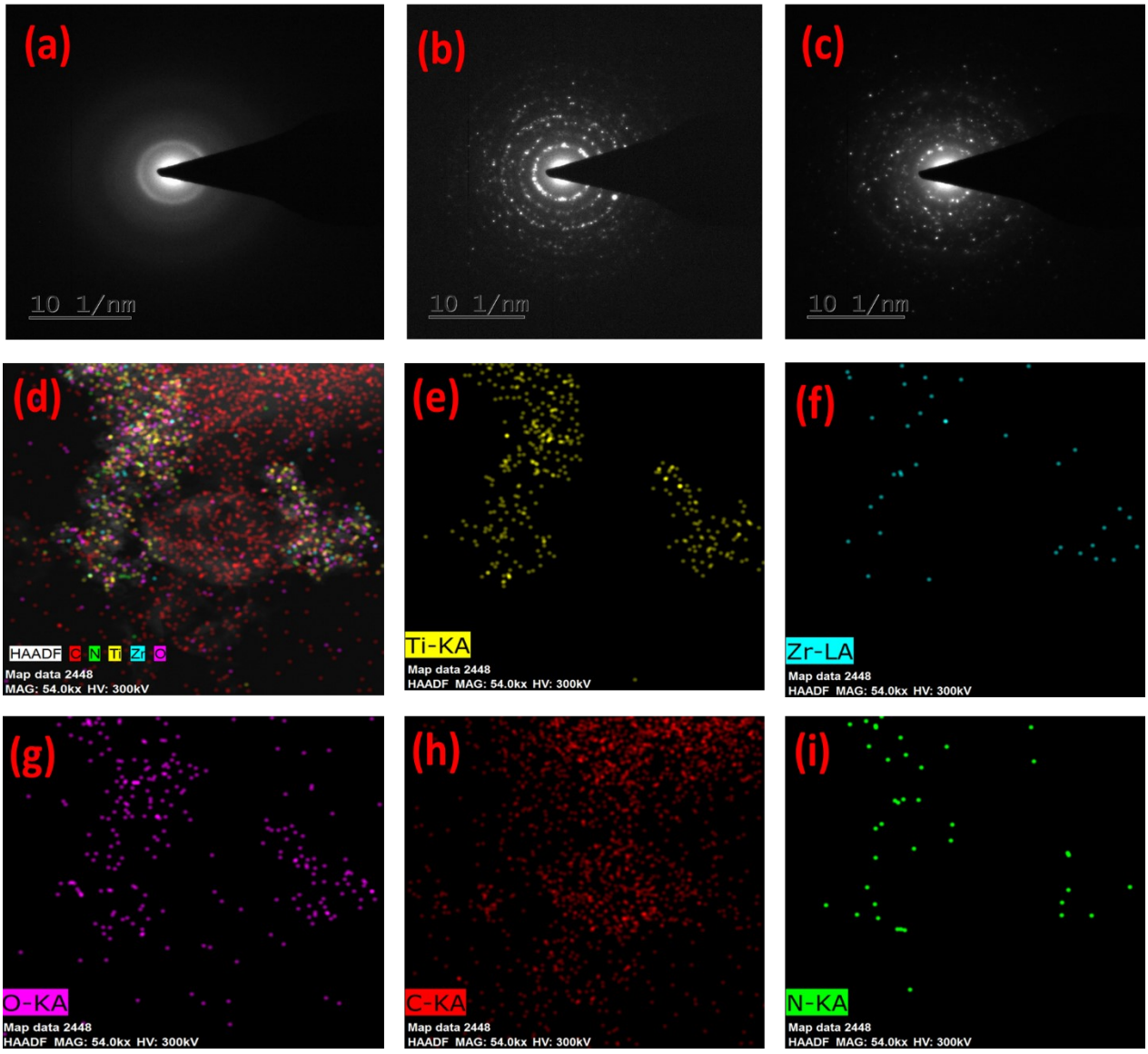


Figure S3. EDS mapping of synthesized TNZ-10-CN provides elemental composition and distribution throughout the material.

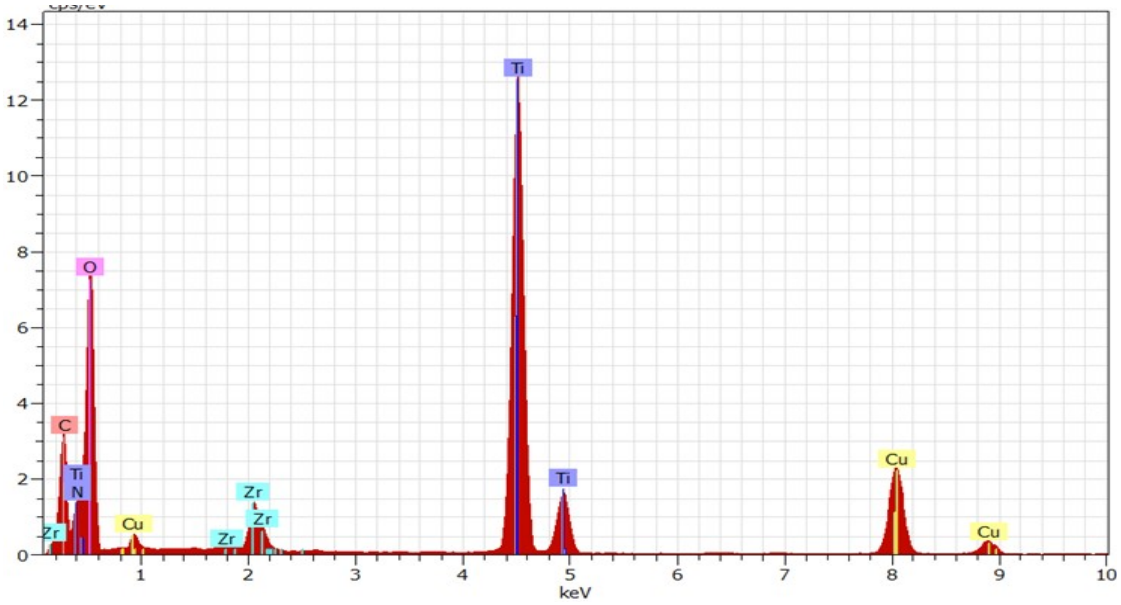


Figure S4. EDX (energy-dispersive X-ray) analysis shows constituent elements in the material.

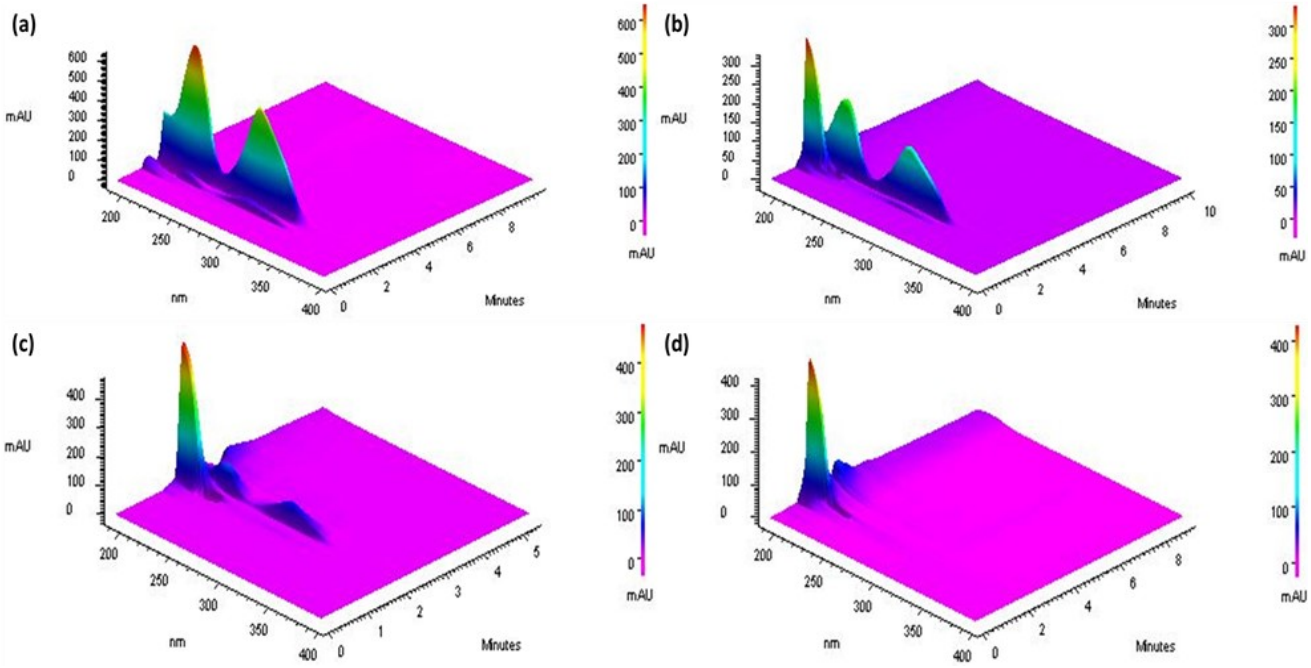
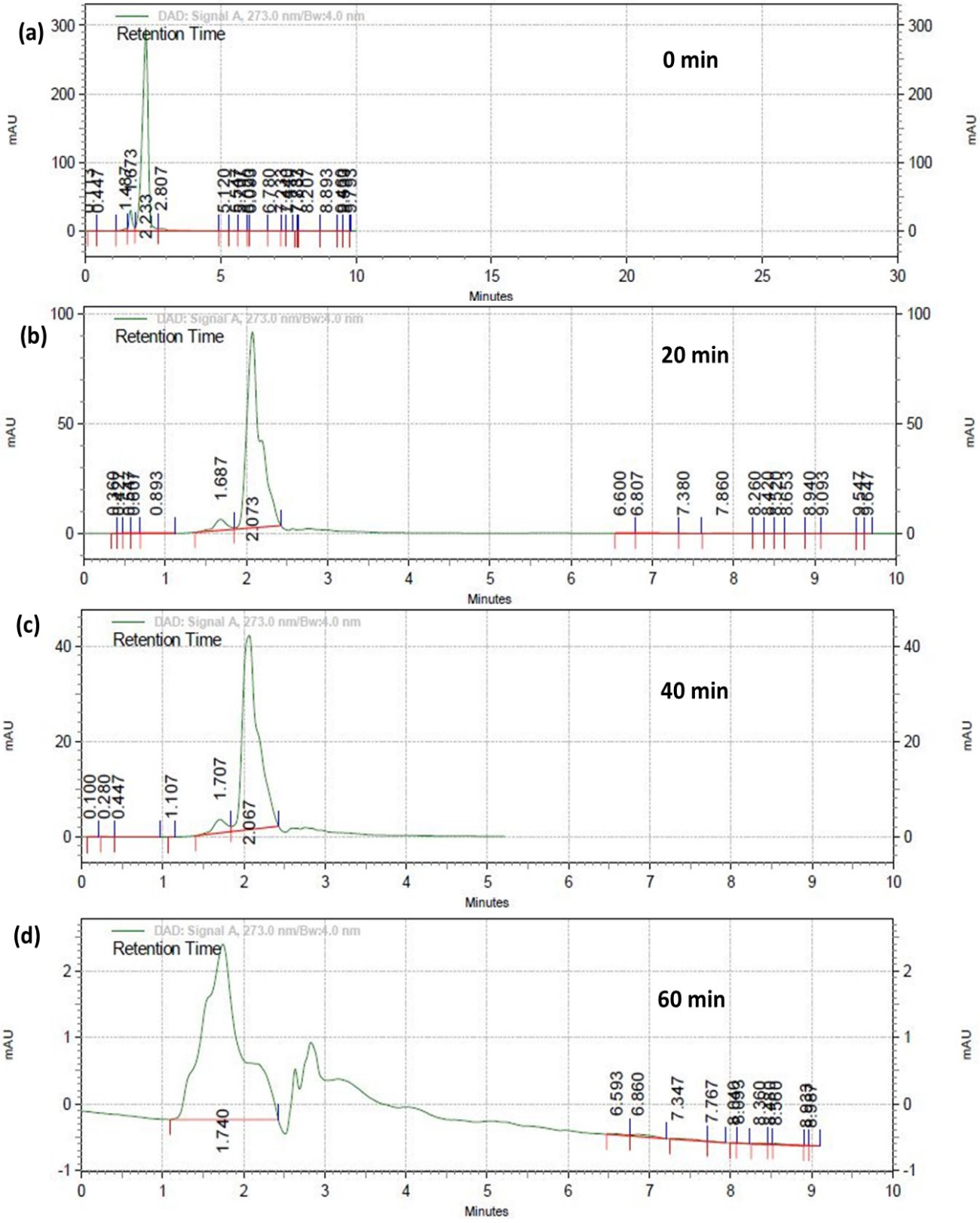


Figure S5. 3D representation of Bromoxynil degradation through HPLC-UV displays retention time-wavelength plot. Graphs (a), (b), (c), and (d) are the degradation results of samples withdrawn after 0 min, 20 min, 40 min, and 60 min of light irradiation.


(a)
DAD: Signal A, 273.0 nm/Bw:4.0 nm
Retention Time
0 min
mAU
Minutes
(b)
DAD: Signal A, 273.0 nm/Bw:4.0 nm
Retention Time
20 min
mAU
Minutes
(c)
DAD: Signal A, 273.0 nm/Bw:4.0 nm
Retention Time
40 min
mAU
Minutes
(d)
DAD: Signal A, 273.0 nm/Bw:4.0 nm
Retention Time
60 min
mAU
Minutes

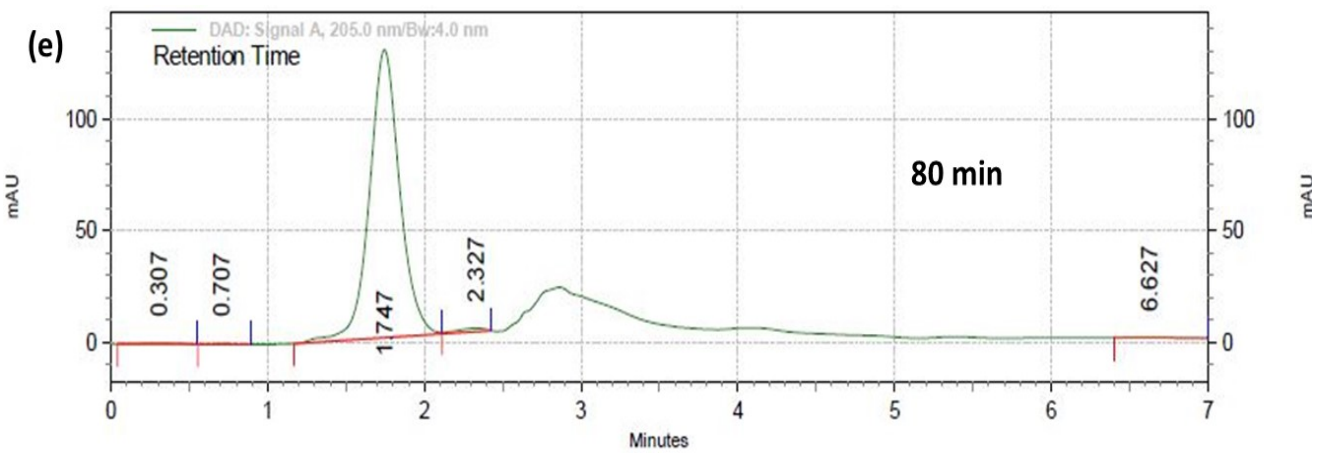


Figure S6. HPLC-UV plot of samples withdrawn after 0min, 20min, 40min, 60min, and 80min of time intervals respectively.

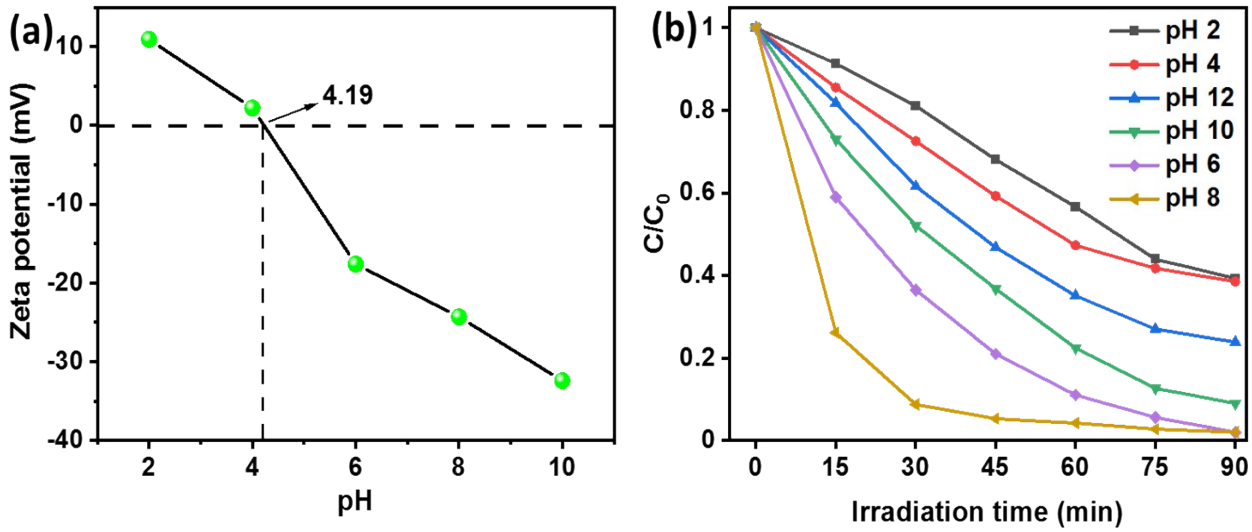


Figure S7(a) Zeta potential of active material TNZ-10-CN, (b) degradation of bromoxynil at different pH.

Table 1. The different weight ratios of doped titania (TNZ-x) and g-C_3N_4 (CN) along with their degradation efficiency (%).

Catalyst	Weight Ratio	Degradation (%)
	1:2	83.46
TNZ-10-CN	**1:4**	**98.70**
	1:6	90.83
	1:2	54.61
TNZ-20-CN	1:4	60.72
	1:6	58.13
	1:2	51.57
TNZ-30-CN	1:4	56.46
	1:6	55.80

The apparent quantum efficiency of H_2 evolution should be measured.

Calculation of apparent Quantum efficiency:

$$Apparent\ Conversion\ efficiency\ (\%) = \frac{Stored\ Chemical\ Energy\ (SCE)}{energy\ of\ incident\ light\ (EIL)}\ X\ 100$$

$$Stored\ Chemical\ Energy\ (SCE) = \frac{N(H_2)}{t}\Delta H_C$$

$$= Moles\ of\ H_2\ produced\ per\ second\ \times\ \Delta H_C$$

$$N(H_2) = moles\ of\ H_2\ produced\ during\ the\ reaction$$

$$t\ =\ duration\ of\ the\ reaction\ (sec)$$

$$\Delta H_C = combustion\ heat\ of\ H_2\ (kJ/mol)$$

$$= 0.0376\ \mu mol \sec^{-1}\ \times\ 285.8\ kJ/mol\left(H_2 = 2H^+ + \frac{1}{2}O_2; \Delta H_C = 285.8\frac{kJ}{mol}\right)$$

$$= 0.01077\ J/sec$$

$$Incident\ light\ intensity\ (ILI) = \frac{Q_i}{4\pi r^2}$$

$$= \frac{250\ W}{4\ \times 3.141\ \times (4)^2} = 1.243\ W/cm^2$$

$$Q_i = 150\ W,\ r = 4\ cm\ (distance\ between\ catalyst\ surface\ and\ lamp)$$

$$Apparent\ Conversion\ efficiency\ (\%) = \frac{0.01077\ J/sec}{1.243\ W/cm^2}\ X\ 100$$

$$= 0.866\ \%$$

The apparent quantum efficiency of H_2 conversion rection has cropped up to 0.86%.

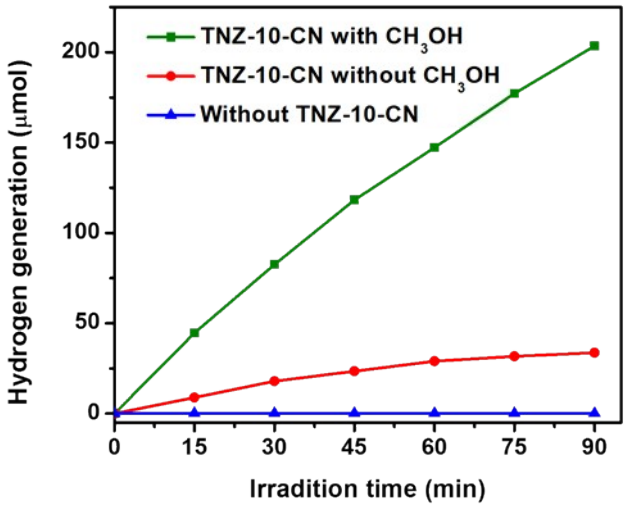


Figure S8. The comparative study of photocatalytic H_2 evolution without CH_3OH in the presence of catalyst TNZ-10-CN under visible light and the H_2 evolution without catalyst under visible light irradiation