Supplementary Material for Charge Transport Phenomena in Heterojunction Photocatalysts: the WO_3/TiO_2 System as an Archetypical Model

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TABLE S1: Parameters used in numerical computations [1–5]

Parameter	Value
TiO_2 Bandgap Energy (eV)	3.2
TiO_2 Electron Affinity (eV)	5.1
TiO_2 Dielectric Constant	41.4
TiO_2 Electron Effective Mass	10
TiO_2 Hole Effective Mass	0.8
TiO_2 Bulk Electron Concentration (cm^{-3})	10^{18}
TiO_2 Absorption Co-efficient, α (cm^{-1})	9.9×10^3
WO_3 Bandgap Energy (eV)	2.74
WO_3 Electron Affinity (eV)	4.91
WO_3 Dielectric Constant	50
WO_3 Electron Effective Mass	2.4
WO_3 Hole Effective Mass	2.4
WO_3 Bulk Electron Concentration (cm^{-3})	10^{19}
WO_3 Absorption Co-efficient, α (cm^{-1})	1.02×10^5
Wavelength (nm)	365
UVA Intensity (mW cm^{-2})	3.15
β_n	1
β_p	1
Saturation Velocity (cm s^{-1}), $V_{sat} = \frac{2.4\times10^2}{1+0.8exp\left[\frac{T}{600}\right]}$	1.03×10^2

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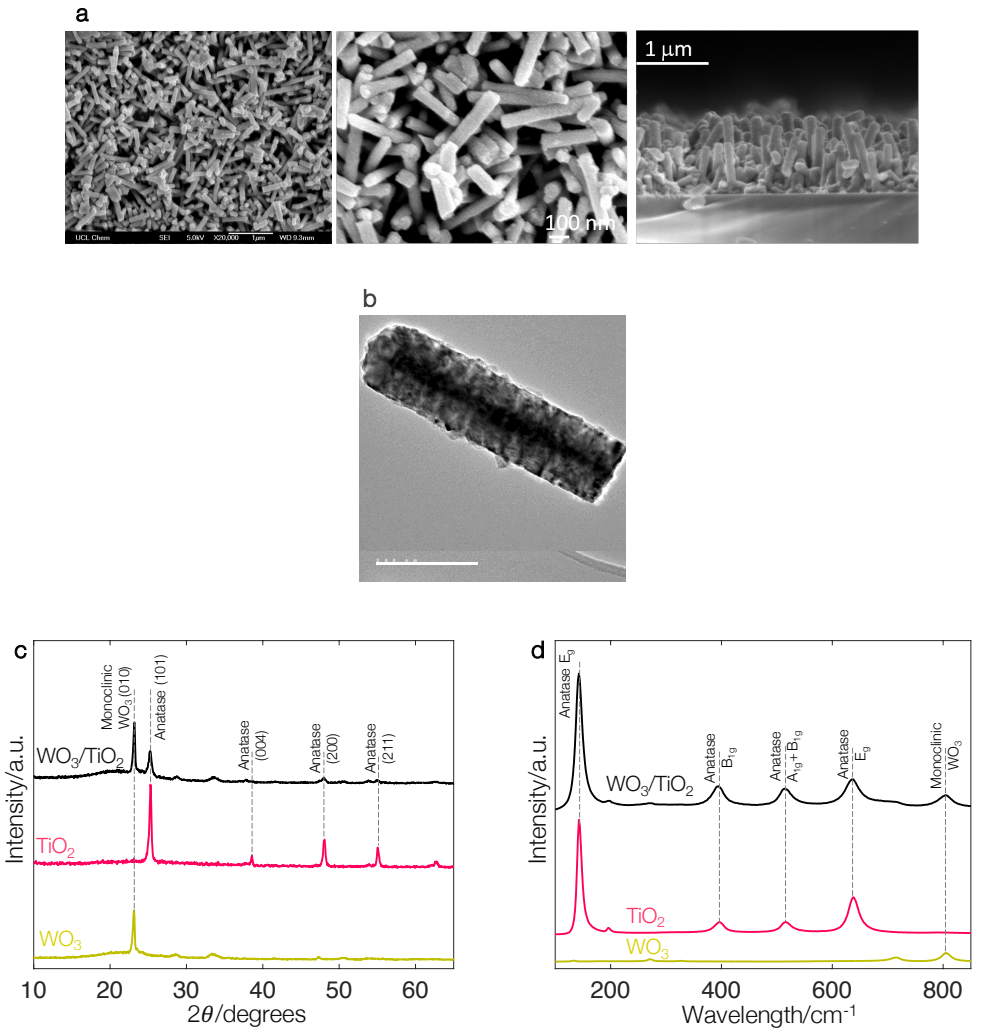

FIG. S1: (a) Scanning electron microscopy (SEM) image and (b) Transmission electron microscopy (TEM), (c) X-ray diffraction patterns of the WT heterojunction film, WO_3 nanorods and anatase TiO_2 (λ = 1.54 A), (d) Raman spectroscopy analysis showing the presence of pure anatase TiO_2 and monoclinic WO_3 phases. [1]

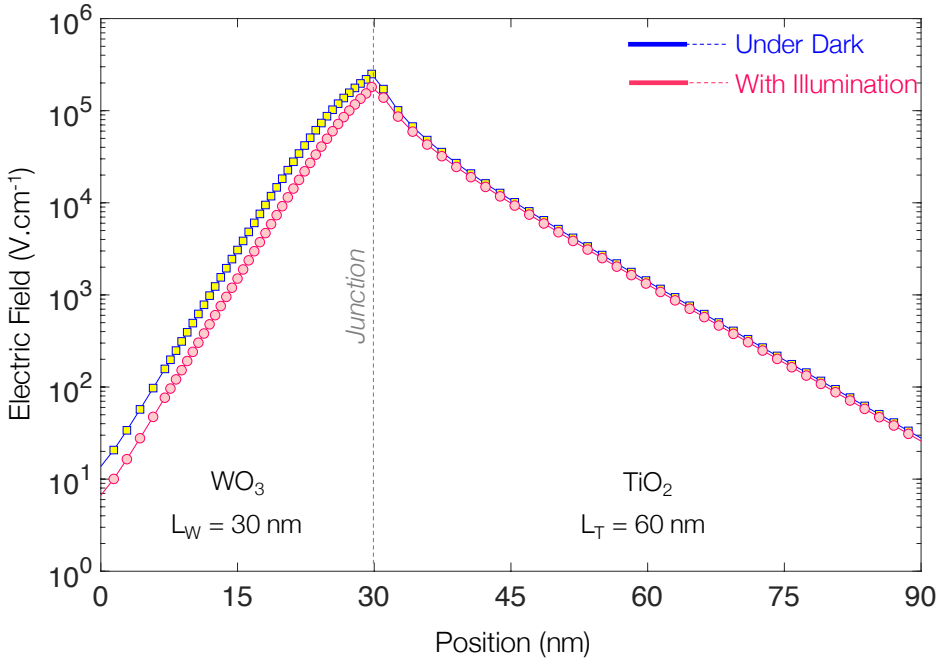

FIG. S2: Calculated electric fields under dark (marked in blue) and UV illumination (marked in red) for the WT junction with $L_W = 30$ nm and $L_T = 60$ nm.

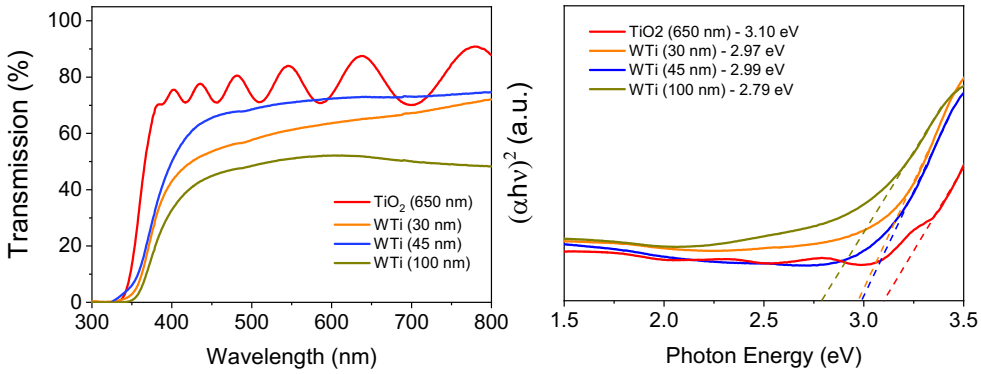

FIG. S3: (a) Absorptance spectra and (b) Tauc plot of WT heterojunctions with different TiO_2 thickness.

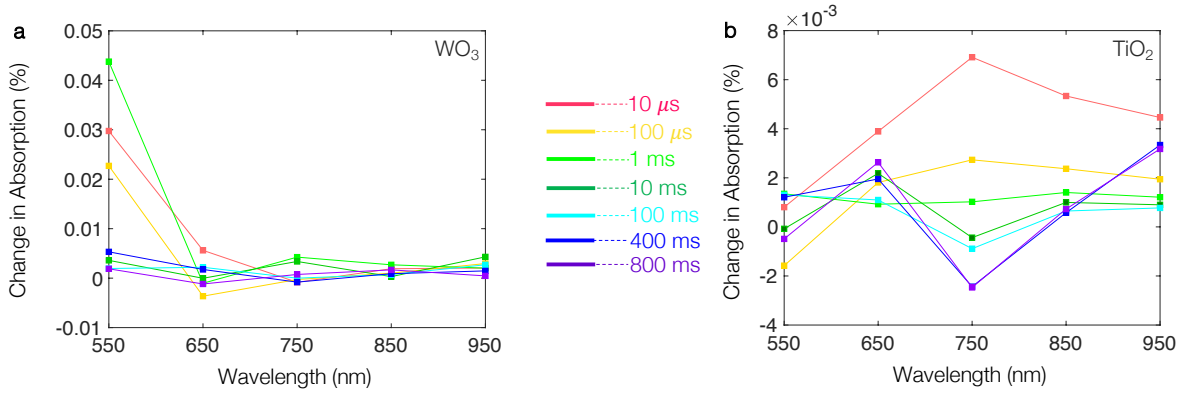

FIG. S4: Transient absorption spectra (probed from 550 to 950 nm) of WO_3 (a) and TiO_2 (b). Samples were excited with a 365 nm laser pulse (1.2 mJ cm^{-2} per pulse, 0.65 Hz pulse rate). ΔA is measured from 10 μs $\rightarrow$ 800 ms after the laser pulse excitation.

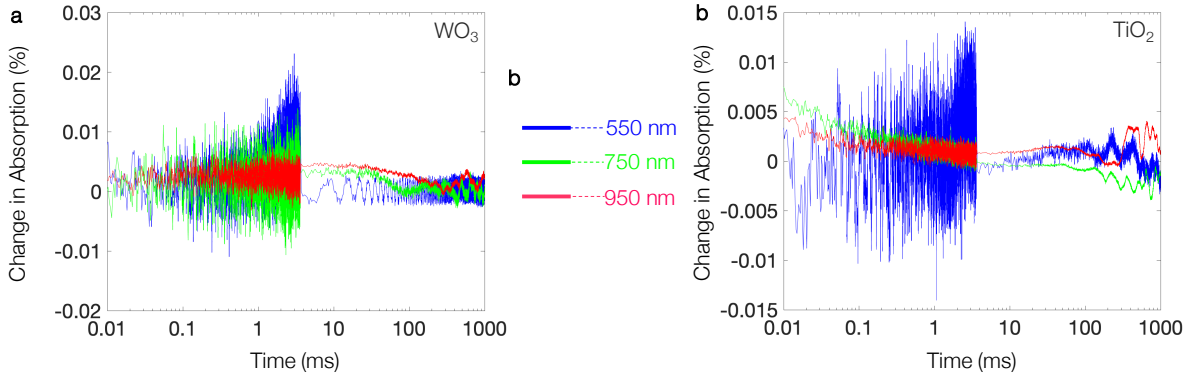

FIG. S5: Transient absorption decay kinetics probed at various wavelengths (550 nm $\rightarrow$ 950 nm) of WO_3 (a) and TiO_2 (b). Samples were excited with a 365 nm laser pulse (1.2 mJ cm^{-2} per pulse, 0.65 Hz pulse rate).