

Supplementary Materials

Efficient and Stable Degradation of Triazophos Pesticide by TiO₂/WO₃ Nanocomposites with S-Scheme Heterojunctions and Oxygen Defects

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1. Experimental

1.1. Equations

The band gap (E_g), valence band (E_{VB}) and conduction band (E_{CB}) of the photocatalysts can be obtained from the following equation (Eq.)

$$\alpha(h\nu) = A(h\nu - E_g)^{1/2} \quad (S1)$$

$$E_{VB} = X - E^e + 0.5E_g \quad (S2)$$

$$E_{CB} = E_{VB} - E_g \quad (S3)$$

Here, α is the absorption coefficient, h represents Planck constant, ν represents light frequency and A is a constant. E^e is a constant with a value of 4.5 eV. The X values of WO₃, TiO₂ are 6.59 and 5.81 eV, respectively.

1.2. DFT calculations

We use density functional theory (DFT) to describe plane wave expansion of wave function, pseudopotential description of electron-nucleus interaction and first-principle pseudopotential of electron-electron interaction. We used CASTEP (Cambridge Serial Total Energy Package) in materials studio to calculate. The generalized gradient approximation (GGA) proposed by Perdew-Burke-Ernzerhof (PBE) is used to deal with forward variations and related interactions. The convergence accuracy is set to Fine. The energy cutoff was set as 400 eV. A vacuum layer of 20 Å was constructed to eliminate interactions between periodic structures of surface models. Other parameters use default values.

Table S1. The amounts of chemicals for preparing WO and TO/WO nanocomposites.

Samples	TiO ₂ (mg)	WCl ₆ (mg)	C ₃ H ₈ O (ml)
80-TO/WO	200	87.2	35
60-TO/WO	200	232.52	35
40-TO/WO	200	523.16	35
WO ₃	0	0.5	35

Table S2. This work is compared with the work in the literature.

Catalyst	Pollutant	Light source	Catalyst dosage	Degradation	literature
N-doped TiO ₂	Diazinon	350 W Xe lamp	2.5 g/L	85 %	[43]
Cu-ZnO	Chorpyriphos	Sunlight irradiation	3 g/L	81 %	[44]
CS/g-C ₃ N ₄	Chorpyriphos	300 W Xe lamp 75 GaN LEDs emitting	0.002 g/L	85 %	[45]
CNS-ZnO	Diazinon	UVA, λ=385 nm	0.1 g/L	53.4 %	[46]
ZnO-SiO ₂ @Fe ₃ O ₄	Malathion	8 W UV-C lamp, λ = 254 nm	0.3 g/L	79.3 %	[47]
N, S-codoped TiO ₂	Tris(2-chloroisopropyl) phosphate	Xenon lamp (2.2 kW), λ > 290 nm	250 mg/L	35 %	[48]
In ₂ S ₃ /BiVO ₄	Glyphosate	125 W, λ > 400 nm mercury lamp	0.4 g/L	74.66 %	[49]
60-TO/WO	Triazophos	300 W Xe lamp	1 g/L	78%	This work