

Supporting Information

An advanced Ag-based photocatalyst Ag₂Ta₄O₁₁ with outstanding activity, durability and universality for removing organic dyes

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The band edge of photocatalyst can be estimated according to the equations $\alpha h\nu = A(h\nu - E_g)^{n/2}$,¹ in which α , ν , A and E_g are absorption coefficient, light frequency, proportionality constant and band gap, respectively. $n = 1$ and $n = 4$ decide the characteristics of the direct and indirect transition in the semiconductor. Using an approximate E_g value (3.95 eV) and the plot of $\ln(\alpha h\nu)$ vs $\ln(h\nu - E_g)$, we deduce the slope of Ag₂Ta₄O₁₁ is about equal to 1 and the corresponding value of n is 2. It indicates the Ag₂Ta₄O₁₁ samples exhibit the indirect band gap as well as direct transition characteristics.² Therefore, as shown the plots of $(\alpha h\nu)^{2/n}$ vs $h\nu$, when $n = 4$ and $n = 1$, the indirect and direct band gaps of Ag₂Ta₄O₁₁ are 3.82 eV and 4.04 eV, respectively.

The band positions of Ag₂Ta₄O₁₁ can be calculated by the following empirical formulae:

$$E_{CB} = X - E_c - 1/2E_g$$

$$E_{VB} = E_{CB} + E_g$$

where X is the absolute electronegativity of the atom semiconductor, expressed as the geometric mean of the absolute electronegativity of the constituent atoms, which is defined as the arithmetic mean of the atomic electron affinity and the first ionization energy; E_c is the energy of free electrons of the hydrogenscale (4.5 eV); E_g is the band gap of the semiconductor; E_{CB} is the conduction band potential and E_{VB} is the valence band potential. The values of X , E_g , E_{CB} , and E_{VB} of the Ta₂O₅ and Ag₂Ta₄O₁₁ samples are shown in Table S1.

Table S1 X , E_g , E_{CB} , and E_{VB} of Ag₂Ta₄O₁₁ and Ta₂O₅ samples

Semiconductor	X (eV)	E_g (eV)	E_{CB} (eV)	E_{VB} (eV)
Ag ₂ Ta ₄ O ₁₁	6.14	3.82	-0.27	3.55
Ta ₂ O ₅	6.34	4.00	-0.16	3.84

Mott-Schottky relationships on n-type and p-type semiconductors are expressed according to the following equations:

$$\frac{1}{C^2} = \left(\frac{2}{\epsilon_0 \epsilon \epsilon_0 N_d} \right) \left[(E - E_{fb}) - \frac{KT}{e_0} \right], \text{ for n type}$$

$$\frac{1}{C^2} = \left(\frac{2}{\epsilon_0 \epsilon \epsilon_0 N_a} \right) \left[(-E + E_{fb}) - \frac{KT}{e_0} \right], \text{ for p type}$$

Where C is the depletion-layer capacitance per unit surface area, N_d and N_a are the donor and acceptor densities, respectively, ϵ_0 is the permittivity of vacuum, ϵ is the dielectric constant of the semiconductor, E is the electrode potential, E_{fb} is the flat-band potential, and KT/e_0 is the temperature dependent term in the Mott-Schottky equation.

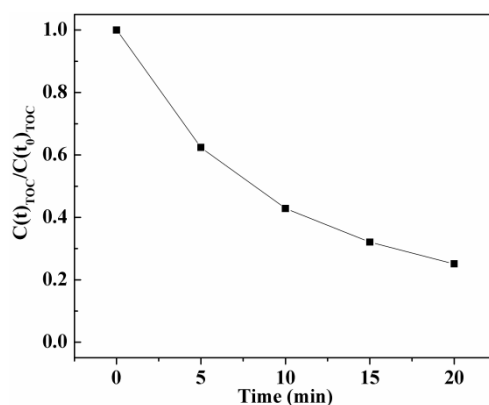


Fig. S1 Dynamic curves of TOC concentrations in the degrading MB over the $Ag_2Ta_4O_{11}$ sample under UV-visible light.

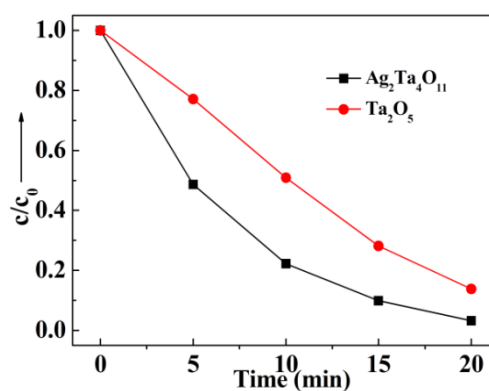


Fig. S2 Dynamic curves of RhB solution over the $Ag_2Ta_4O_{11}$ and Ta_2O_5 samples under UV-visible light.

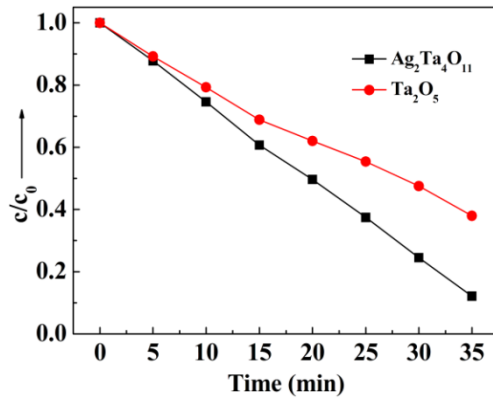


Fig. S3 Dynamic curves of MO solution over the Ag₂Ta₄O₁₁ and Ta₂O₅ samples under UV-visible light.

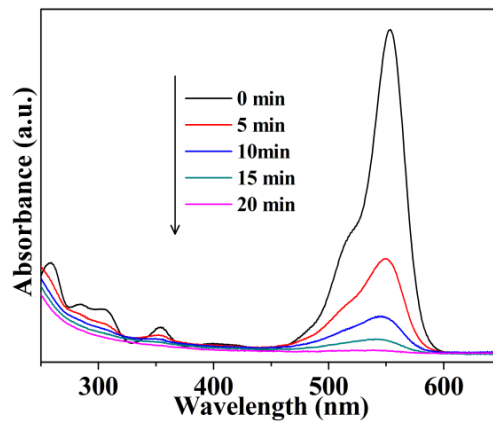


Fig. S4 Absorbance variations of RhB solution over the Ag₂Ta₄O₁₁ sample under UV-visible light.

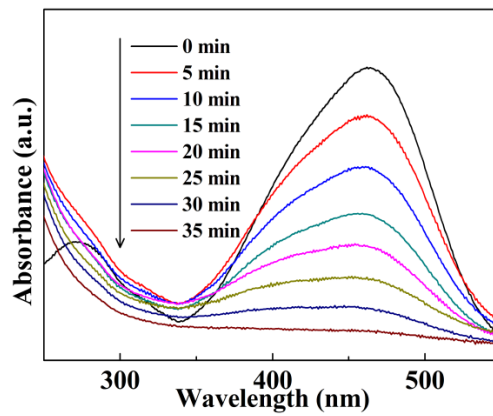


Fig. S5 Absorbance variations of MO solution over the Ag₂Ta₄O₁₁ sample under UV-visible light.

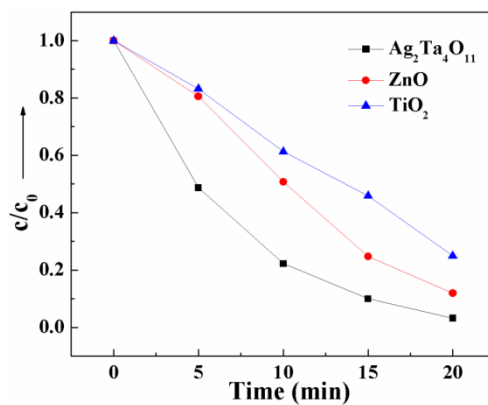


Fig. S6 Dynamic curves of RhB solution over the $\text{Ag}_2\text{Ta}_4\text{O}_{11}$, ZnO and TiO_2 samples under UV-visible light.

Reference

1. M. A. Butler, *J. Appl. Phys.* 1977, **48**, 1914-1920.
2. Z. G. Yi, J. H. Ye, N. Kikugawa, T. Kako, S. X. Ouyang, H. Stuart-Williams, H. Yang, J. Y. Cao, W. J. Luo, Z. S. Li, Y. Liu, and R. L. Withers, *Nat. Mater.*, 2010, **9**, 559-563.