Electronic Supplementary Material (ESI) for CrystEngComm.
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Electronic supporting information (ESI) for

Simultaneous doping and heterojunction of silver on $Na_2Ta_2O_6$ nanoparticles for visible light driven photocatalyst: Relevance between tunable optical absorption, defect chemistry and photocatalytic activity

Tingting Wang, Junyu Lang, Yingjie Zhao, Yiguo Su*, Yanxiao Zhao, Xiaojing Wang*

College of Chemistry and Chemical Engineering, Inner Mongolia University, Hohhot, Inner Mongolia 010021, P. R. China

* Fax:+86-471-4992981; Tel:+86-471-4344579;

cesyg@imu.edu.cn; wang_xiao_jing@hotmail.com.

ESI-1

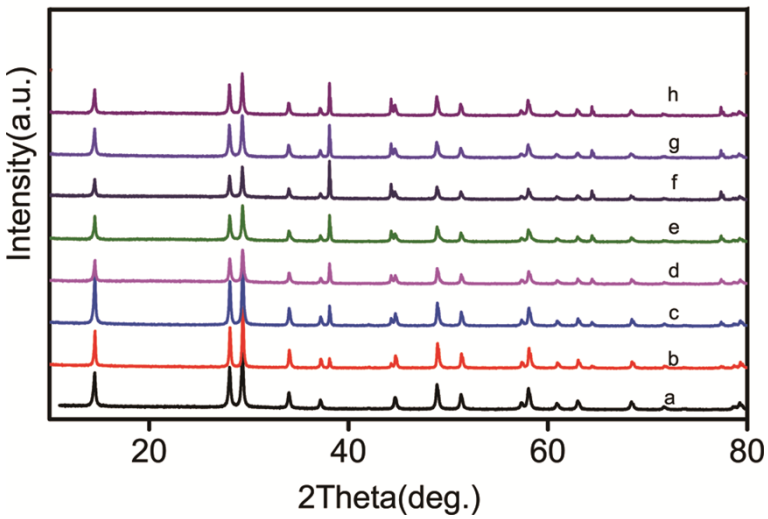

Fig. S1 The XRD patterns of bare $Na_2Ta_2O_6$ (a) and the $Na_2Ta_2O_6$/Ag heterojunction photocatalysts prepared with varied R. R = 0.2 (b), 0.4 (c), 0.6 (d), 0.8 (e), 1.0 (f), 1.2 (g), and 1.4(h).

ESI-2

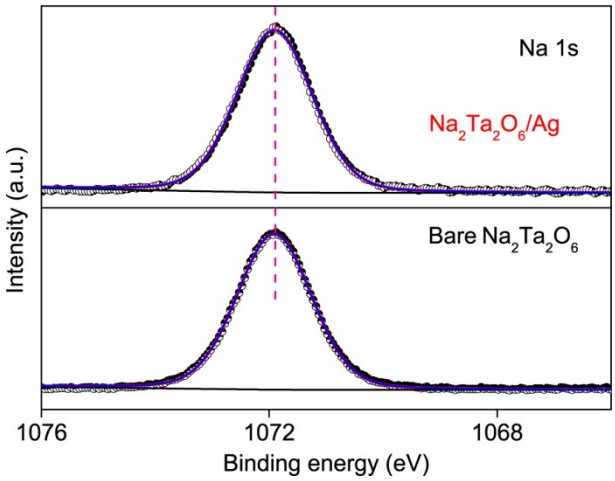

Fig. S2 Na 1s XPS spectra of bare $Na_2Ta_2O_6$ and $Na_2Ta_2O_6$/Ag (with R value of 1.2).

ESI-3

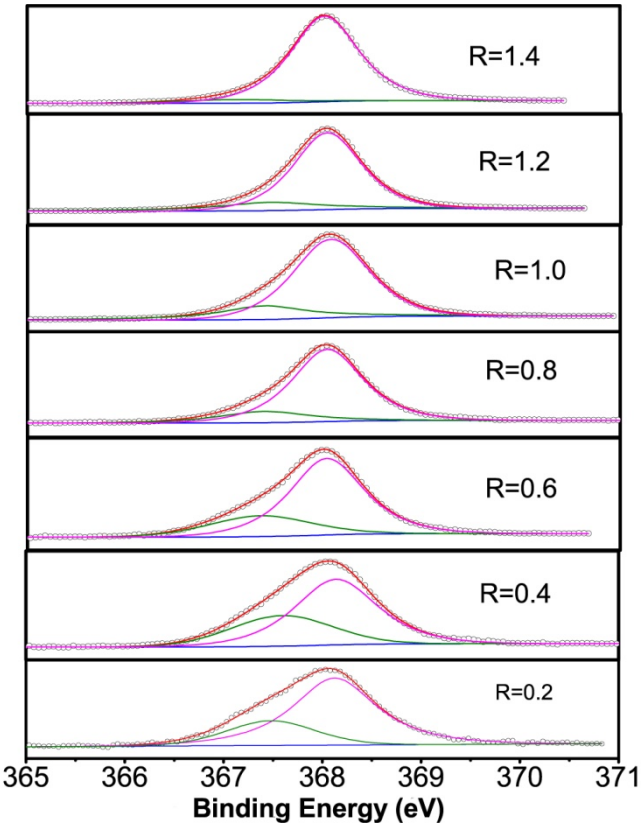

Fig. S3 Ag $3d_{5/2}$ XPS spectra of $Na_2Ta_2O_6$/Ag with different initial Ag/Ta molar ratios.

ESI-4

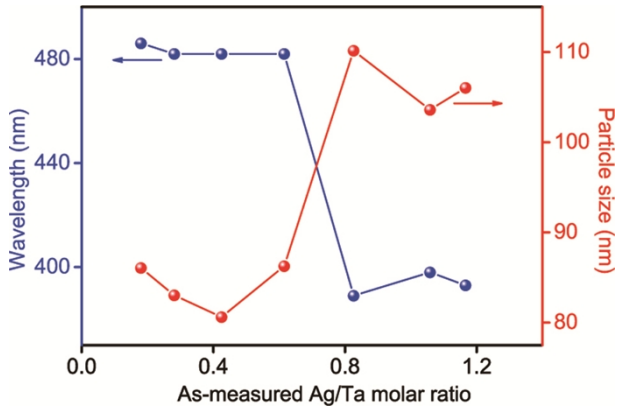

Fig. S4 SPR absorption maximum and XRD calculated particle size as a function of as-measured Ag/Ta molar ratios.

ESI-5

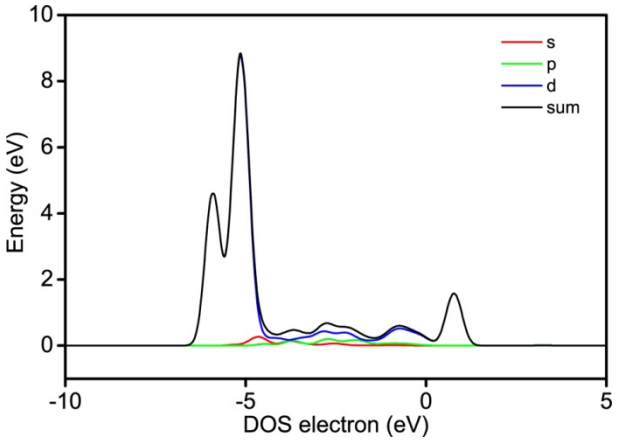

Fig. S5 Density of states (DOS) of Ag in Ag doped $Na_2Ta_2O_6$.

ESI-6

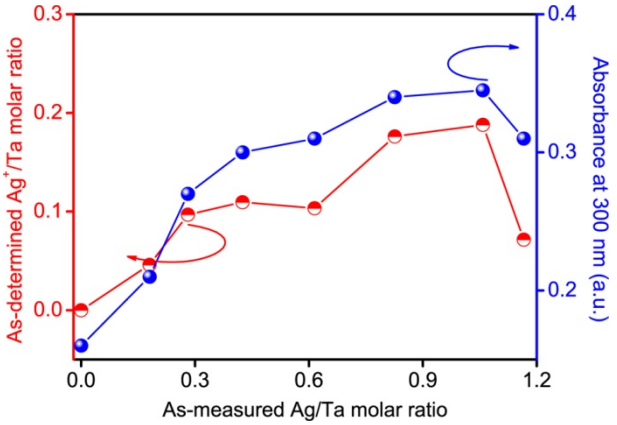

Fig. S6 Correlation between as-determined Ag^{+}/Ta molar ratio and the intensity of the interband absorption at 300 nm as a function of as-measured Ag/Ta molar ratio.

ESI-7

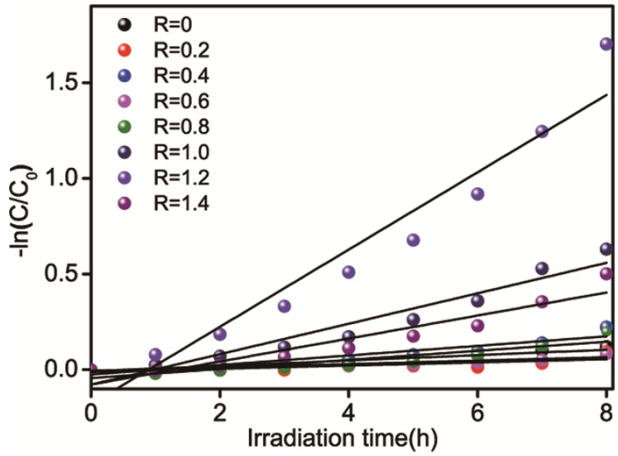

Fig. S7 The $-\ln(C/C_0)$ versus time curves of rhodamine B photodegradation over $Na_2Ta_2O_6$/Ag under visible light irradiation.

ESI-8

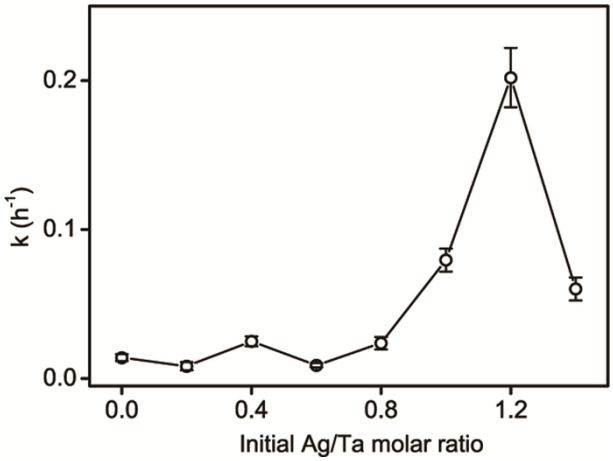

Fig. S8 Rhodamine B degradation rate constant as a function of initial Ag/Ta molar ratio.

ESI-9

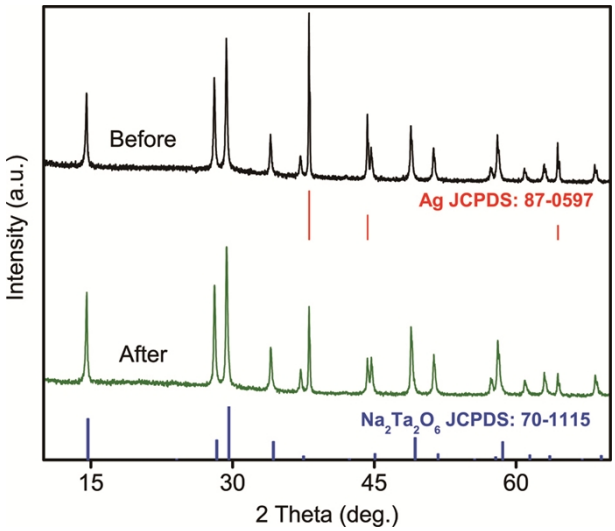

Fig. S9 XRD patterns of $Na_2Ta_2O_6$/Ag heterojunctions before and after photocatalytic degradation reaction.

ESI-10

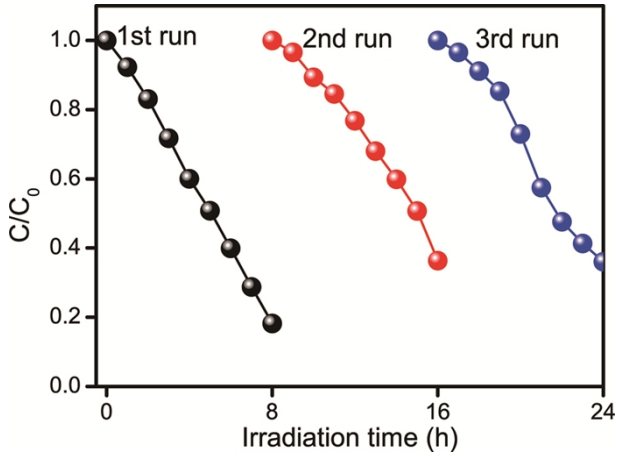

Fig. S10 The cycling runs in the photocatalytic degradation of rhdomine B over $Na_2Ta_2O_6$/Ag heterojunction photocatalyst.

ESI-11

The conduction band edge energy of a semiconductor at the point of zero charge can be expressed by

$$E_{CB} = X - 0.5E_g$$

whereE_{CB} is the conduction band edge potential and X is the Mulliken electronegativity of the semiconductor, which is the geometric mean of the electronegativities of the constituent atoms. E_g is the band gap energy of $Na_2Ta_2O_6$/Ag nanoparticles, which is determined to be ~4.68 eV for initial Ag/Ta molar ratio of 1.2. The Mulliken electronegativity of an atom is the arithmetic mean of the atomic electron affinity and the first ionization energy. According to this expression, the rough conduction band potential was determined to be 2.93 eV with respect to absolute vacuum energy. On the basis of the relationship between the absolute vacuum energy and the normal electrode potential, the conduction band potential was estimated to be -1.57 V vesus NHE.

ESI-12

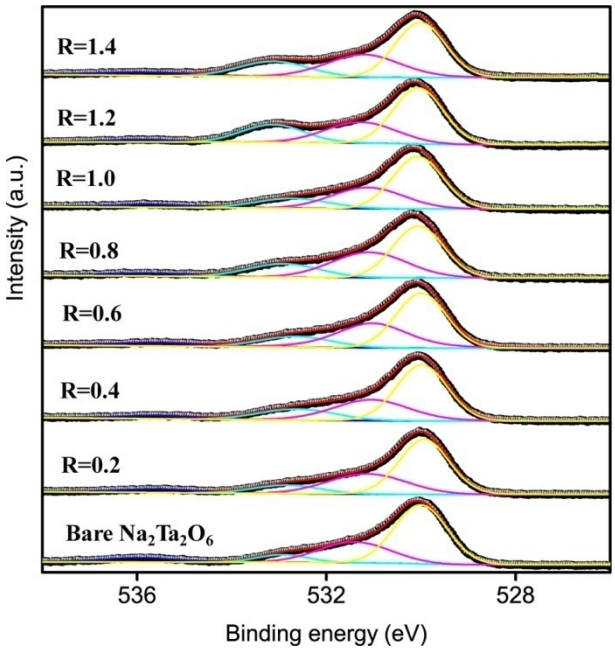

Fig. S11 O 1s XPS spectra of all $Na_2Ta_2O_6$/Ag samples.

ESI-13

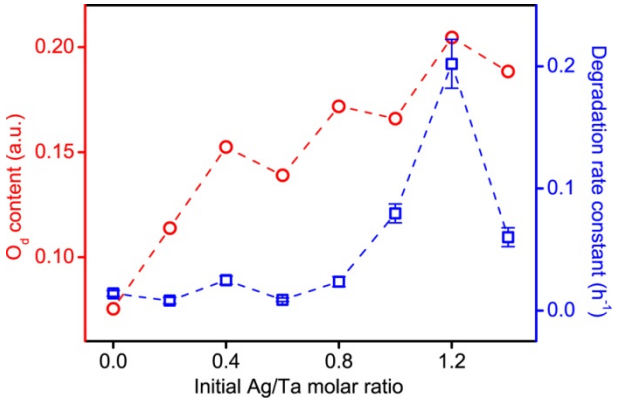

Fig. S12 O_d content and degradation rate constant as a function of initial Ag/Ta molar ratio.

ESI-14

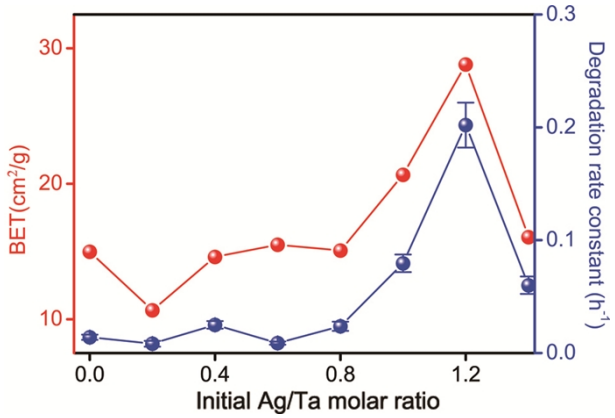

Fig. S13 BET surface area and degradation rate constant as a function of initial Ag/Ta molar ratio.

ESI-15

The photodeposited $Na_2Ta_2O_6$/Ag sample was prepared as follow: The given amount of $Na_2Ta_2O_6$ powder was dispersed in a methyl orange aqueous solution (20 mg/L) in a flask. The solution was constantly stirred using a magnetic stirrer for 1 h at room temperature in dark. Then, the adequate amount of $AgNO_3$ solution was added to the resulted solution and irradiated using a 300 W Xenon (Xe) lamp in atmosphere with stirring for 2 hours. The obtained suspension of particles was collected and dried in a vacuum oven at 60°C.

The physical mixed $Na_2Ta_2O_6$/Ag sample was prepared as follow: Ag nanoparticles were prepared similar to that of $Na_2Ta_2O_6$/Ag. Briefly, given amount of Ag_2O was dissolved in a mixed solution containing 30 mL of NH_4OH and 10 mL NaClO (10%) with vigorous stirring. This suspension was sealed in 100 mL Teflon-lined stainless steel autoclaves and heated in a preheated oven at 220℃ for 48 h. After the autoclave was air-cooled to room temperature naturally, the resultant product was collected by centrifugation and washed with distilled water thoroughly for several times. Finally, the obtained Ag products were dried at 60℃ for 3 h in air. Then given amounts of as-prepared $Na_2Ta_2O_6$ and Ag were mixed together without further heating procedure.

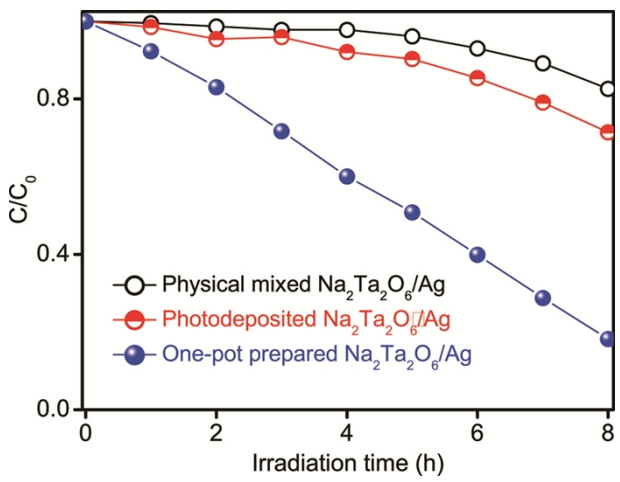

Fig. S14 Rhodamine B degradation photocatalytic performance of $Na_2Ta_2O_6$/Ag prepared with different method.

XPS measurement on physical mixed $Na_2Ta_2O_6$/Ag and photodeposited $Na_2Ta_2O_6$/Ag indicated that no obvious signal belonging Ag^+ ions was observed.

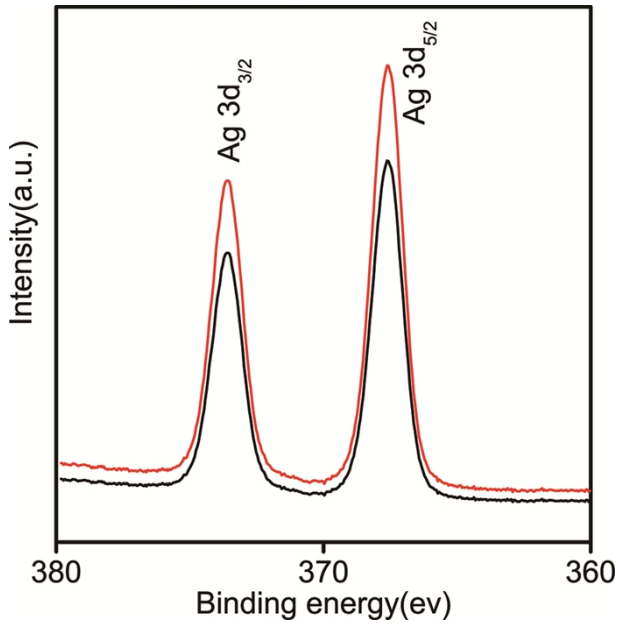

Fig. S15 XPS signal of Ag 3d. The red line indicates photodeposited sample. The black line indicates the physical mixed sample.

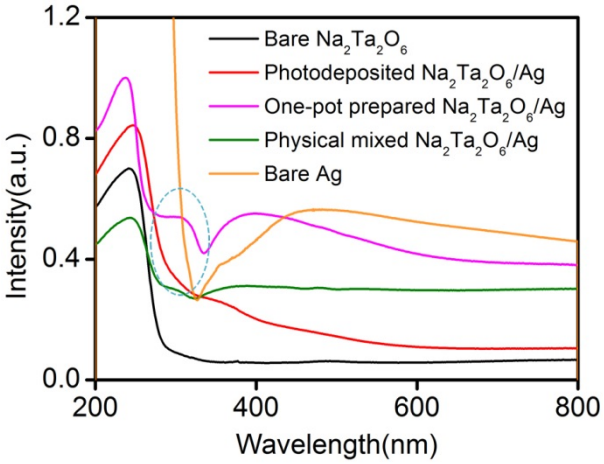

Fig. S16 Optical diffuse reflectance spectra of $Na_2Ta_2O_6$/Ag heterojunctions prepared by different methods.