

## Supporting Information

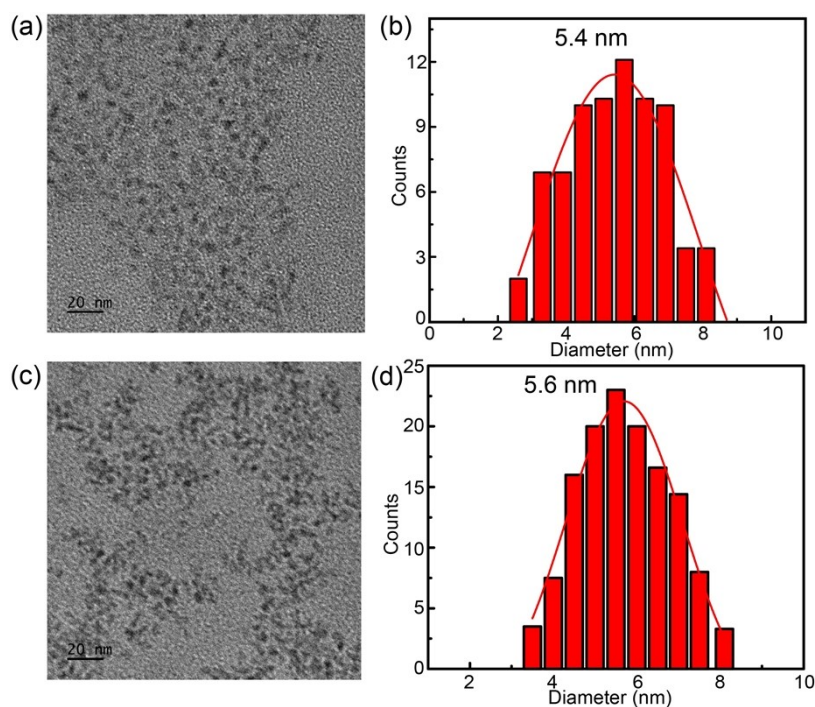
### Triplet Generation at CdTe Quantum Dots/Anthracene Interface Mediated by Hot and Thermalized Electron Exchange for Enhanced Production of Singlet Oxygen

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**Figure S1.** Transmission electron microscopy image of CdTe QDs (a) and CdTe QDs-ACA complexes (c). The size distribution histogram of CdTe QDs (b) and CdTe QDs-ACA complexes (d).

### The binding mode of ACA and QD.

Figure S2 shows the FT-IR spectra of free ACA and CdTe QDs-ACA. We can notice that the absorption modes of C=O stretching and O-H vibration in the carboxylic acid group of ACA are observed at  $1679\text{ cm}^{-1}$  and  $1448\text{ cm}^{-1}$ ,<sup>1, 2</sup> respectively. After ACA is adsorbed onto the surface of CdTe QDs, the peak of C=O stretching mode is slightly shifted to a lower wavenumber of  $1660\text{ cm}^{-1}$ , and the vibration mode of O-H at  $1463\text{ cm}^{-1}$  appears concomitantly. These observations suggest that the ACA is probably anchored to the surface of CdTe QDs through the bridging coordination mode (inset of Figure 1b and Figure S2), which is consistent with the reported results<sup>3, 4</sup>.

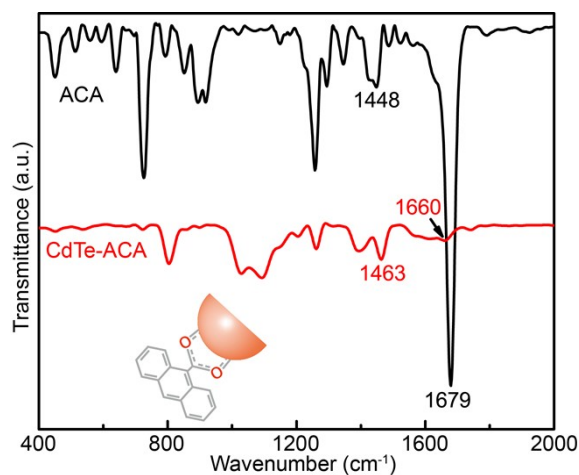


Figure S2. FT-IR spectra of free ACA (black line) and CdTe QDs-ACA (red line).

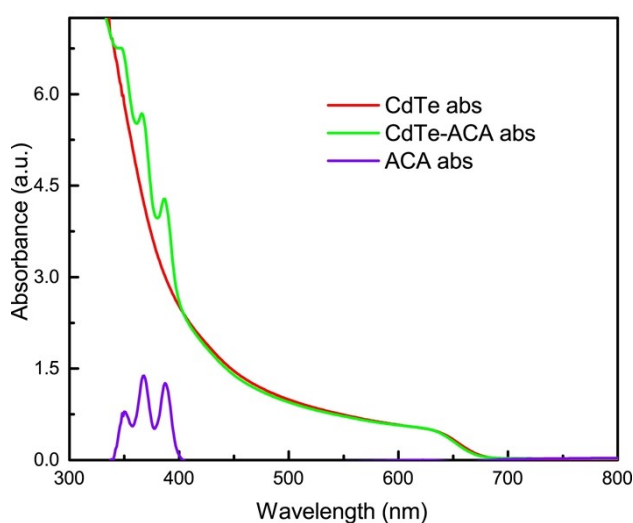
### Calculation of the number of ACA molecules per QD and the concentration of CdTe QDs.

The average number of ACA molecules ( $n$ ) per CdTe QDs can be estimated from the absorption spectrum (Figure S2) using the extinction coefficient reported for CdTe QDs ( $358540 \text{ M}^{-1} \text{ cm}^{-1}$  at  $640 \text{ nm}$ )<sup>5</sup> and ACA ( $6400 \text{ M}^{-1} \text{ cm}^{-1}$  at  $386 \text{ nm}$ )<sup>6</sup> according to the equation of  $n = [A(\text{ACA})/\epsilon(\text{ACA})]/[A(\text{QD})/\epsilon(\text{QD})]$ <sup>7</sup>, where  $A$  and  $\epsilon$  is the absorbance and extinction coefficient, respectively. Then, we can calculate that the average number of ACA molecules ( $n$ ) bound to each CdTe QDs is around 155.

As previous reported<sup>5</sup>, the concentration of CdTe QDs (C) can be calculated using Lambert-Beer's law:

$$C = \frac{A}{\varepsilon L}$$

where A is the absorbance of the first exciton absorption peak,  $\varepsilon$  is the extinction coefficient per mole of QDs, L is the path length (cm) of the radiation beam used for recording the absorption spectrum. L is 1cm in our experiment. Then, the concentration of CdTe QDs with a value of  $1.26 \times 10^{-6}$  mol/L was obtained. As shown in Figure 1b, the absorbance of the exciton peak of CdTe QDs is well maintained upon the ACA functionalization. Therefore, the concentration of CdTe QDs-ACA complex is equal to that of CdTe QDs ( $1.26 \times 10^{-6}$  mol/L).



**Figure S3.** Absorption spectra of CdTe QDs (red), CdTe QDs-ACA complexes (green) and ACA (blue). The Absorption spectra of ACA (blue) obtained by subtracting that of CdTe QDs (red) from that of CdTe QDs-ACA complexes (green).

**Dynamics fitting.** The dynamical curve was fitted using a multi-exponential function

as below:

$$I(t) = \sum_i^n A_i \exp\left(-\frac{t}{\tau_i}\right)$$

The average lifetime  $\langle\tau\rangle$  is calculated according to the following equation:

$$\langle\tau\rangle = \frac{\sum_i^n A_i \tau_i}{\sum_i^n A_i}$$

where  $A_i$  represents the percentage of the corresponding lifetime ( $\tau_i$ ).

The TET time constant was calculated as: 
$$\tau_{TET} = \frac{1}{1/\langle\tau_{QD-ACA}\rangle - 1/\langle\tau_{QD}\rangle}$$

The TET yield was calculated according to 
$$\phi_{TET} = 1 - \frac{\langle\tau_{QD-ACA}\rangle}{\langle\tau_{QD}\rangle}$$

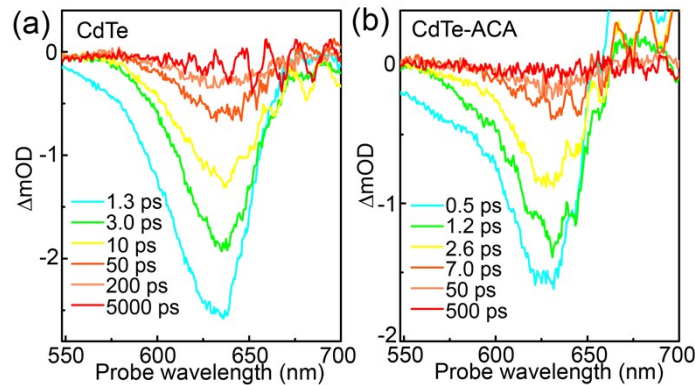
**Table S1. PL lifetime decay parameters of free CdTe QDs and CdTe QDs-ACA complex.**

	$\tau_1/\text{ns}$	$\tau_2/\text{ns}$	$\tau_{av}/\text{ns}$	$\tau_{TET}/\text{ns}$	$\phi_{TET}$
CdTe	0.73±0.02 (73%)	8.91±0.26 (27%)	2.94	/	/
CdTe-ACA	0.46±0.01 (88%)	7.33±0.18 (12%)	1.28	2.27	56%

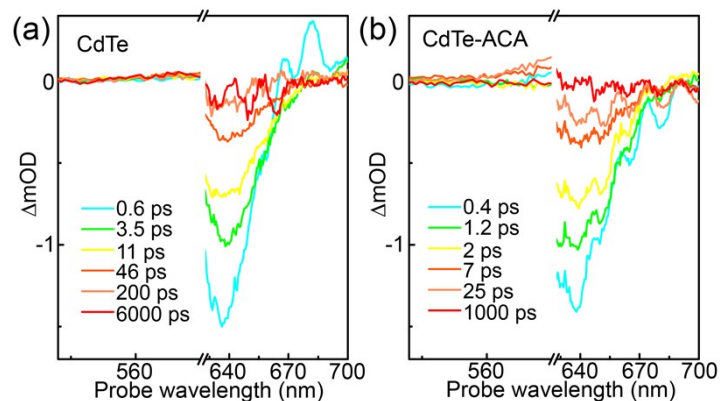
**Table S2. Fitting parameters for the decay curves of free CdTe QDs and CdTe QDs-ACA complex.**

	$\tau_1/\text{ps}$	$\tau_2/\text{ps}$	$\tau_3/\text{ps}$	$\tau_{\text{av}}/\text{ps}$	$\varphi_{\text{TET}}$
CdTe	7.8±0.6 (34%)	165±16 (53%)	6094±600 (13%)	882	/
CdTe-ACA	3.0±0.3 (44%)	35±6 (49%)	1580±300 (7%)	129	85%

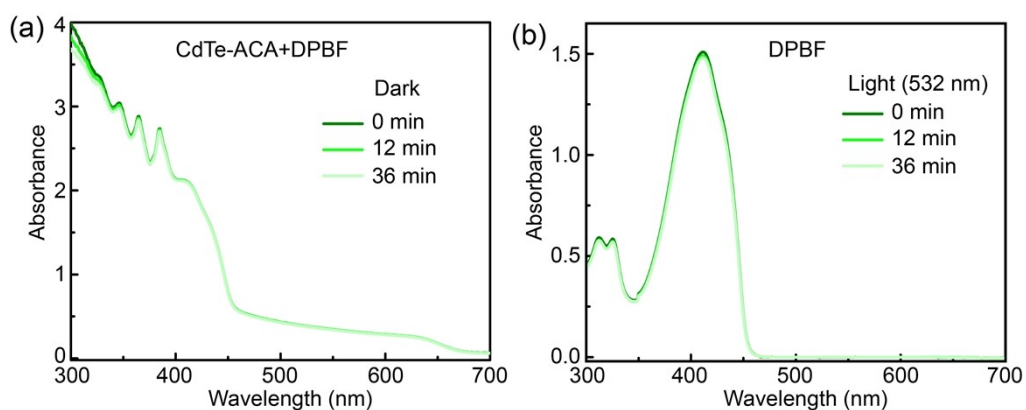
**Calculation of the overall TET efficiency:** The efficiency of hot electron exchange mediated TET was determined to be ~27% with 530 nm excitation. Thus, we can calculate that 73% of the photoexcited electrons relax to the CB edge of CdTe QDs, which is termed as thermalized electrons. In addition, the yield of ~85% from the thermalized electron-exchange mediated TET is estimated according to the average decay lifetimes of free CdTe QDs and CdTe QDs-ACA complexes. As a result, the overall TET efficiency from CdTe QDs to ACA under excitation at 530 nm can be calculated as:  $27\% + (1-27\%) \times 85\% = 89\%$ .



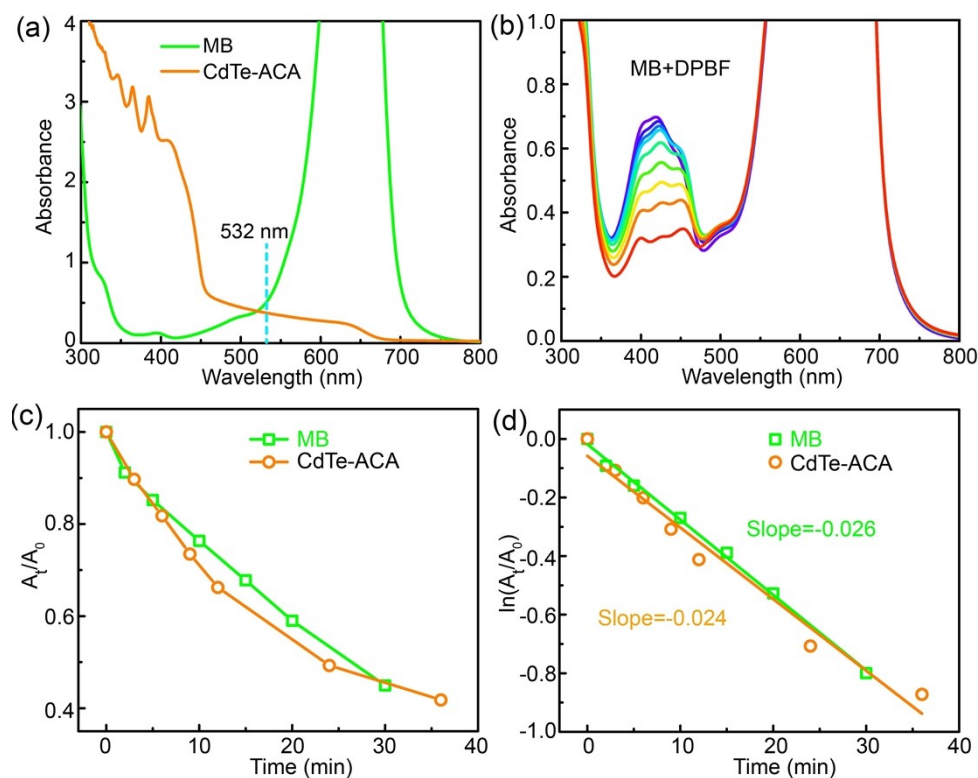
**Figure S4.** TA spectra of free CdTe QDs (a) and CdTe QDs-ACA complex (b) at different time delays with the excitation at 440 nm.



**Figure S5.** TA spectra for free CdTe QDs (a) and CdTe QDs-ACA complex (b) at different time delays under the excitation at 610 nm.



**Figure S6.** (a) Time-dependent absorption spectra of DPBF in the presence of CdTe QDs-ACA complex without the laser irradiation. (b) Time-dependent absorption spectra of DPBF alone under the laser irradiation.



**Figure S7.** (a) Absorption spectra of CdTe QDs-ACA complex in the presence of DPBF and methylene blue (MB) in water as the quantum yield standard. The absorbance of CdTe QDs-ACA and MB are 0.375 and 0.506 at 532 nm, respectively. (b) Time-dependent absorption spectra of DPBF in the presence of MB under 532 nm laser irradiation. Normalized absorbance (c) and degradation kinetics (d) of DPBF in the presence of CdTe QDs-ACA complex and MB.  $A_0$  and  $A_t$  are the characteristic absorbance of DPBF at 407 nm before and after laser irradiation, respectively.

## References

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