

Electronic Supplementary Material (ESI) for Catalysis Science & Technology.
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Supporting Information

High-Efficiency Visible-light Photocatalytic H₂O₂ Production

Using CdSe-based Core/shell Quantum Dots†

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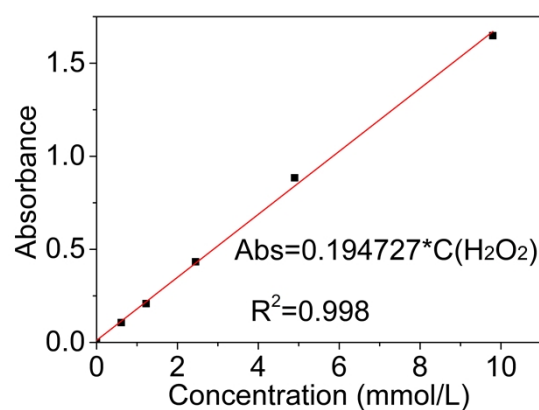


Fig S1. The work curve for determination of H_2O_2 concentration. The calibration curve was prepared by 1 mL of the H_2O_2 solution with quantified concentration and add with 2.0 mL of deionized water and 2.0 mL of titanium potassium oxalate solution (0.05 mol/L). The absorbance of H_2O_2 chromogenic solution was monitored by measuring the absorbance at 400 nm.

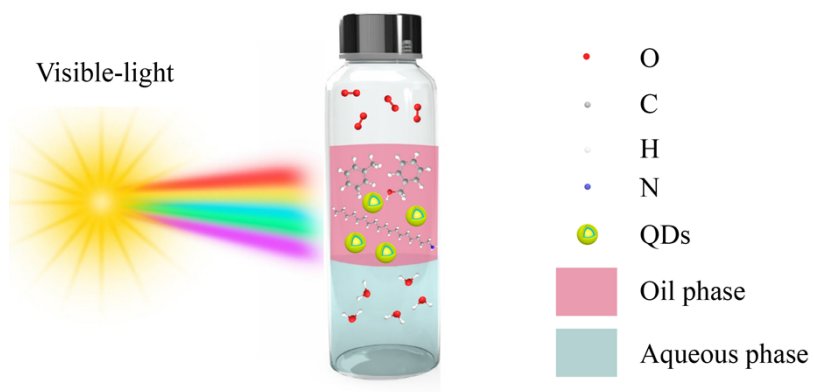


Fig S2. Photocatalytic H_2O_2 production utilizing the two-phase system.

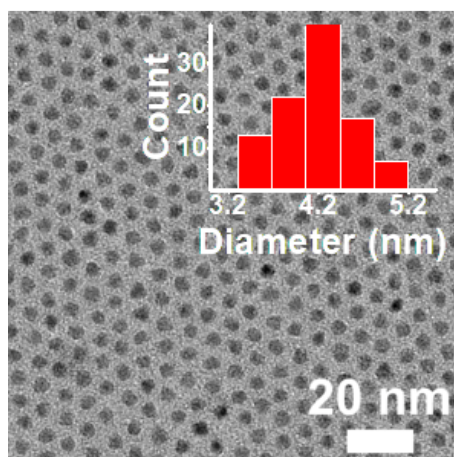


Fig S3. TEM images of CdSe₅₉₀ plain core QDs. Inset: the size distribution histograms of CdSe₅₉₀ plain core QDs.

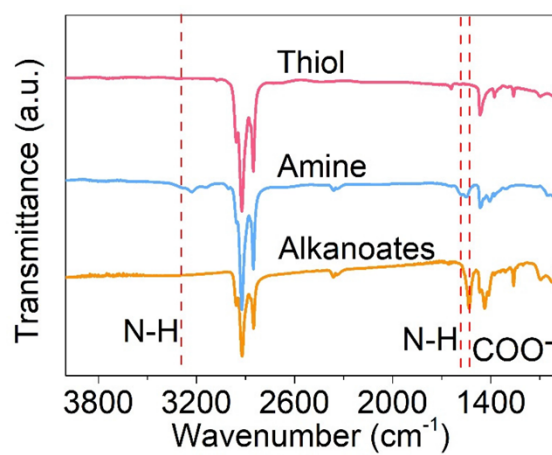


Fig S4. FT-IR spectra of thiol-, amine-, alkanates-coated CdSe₅₅₀ QDs.

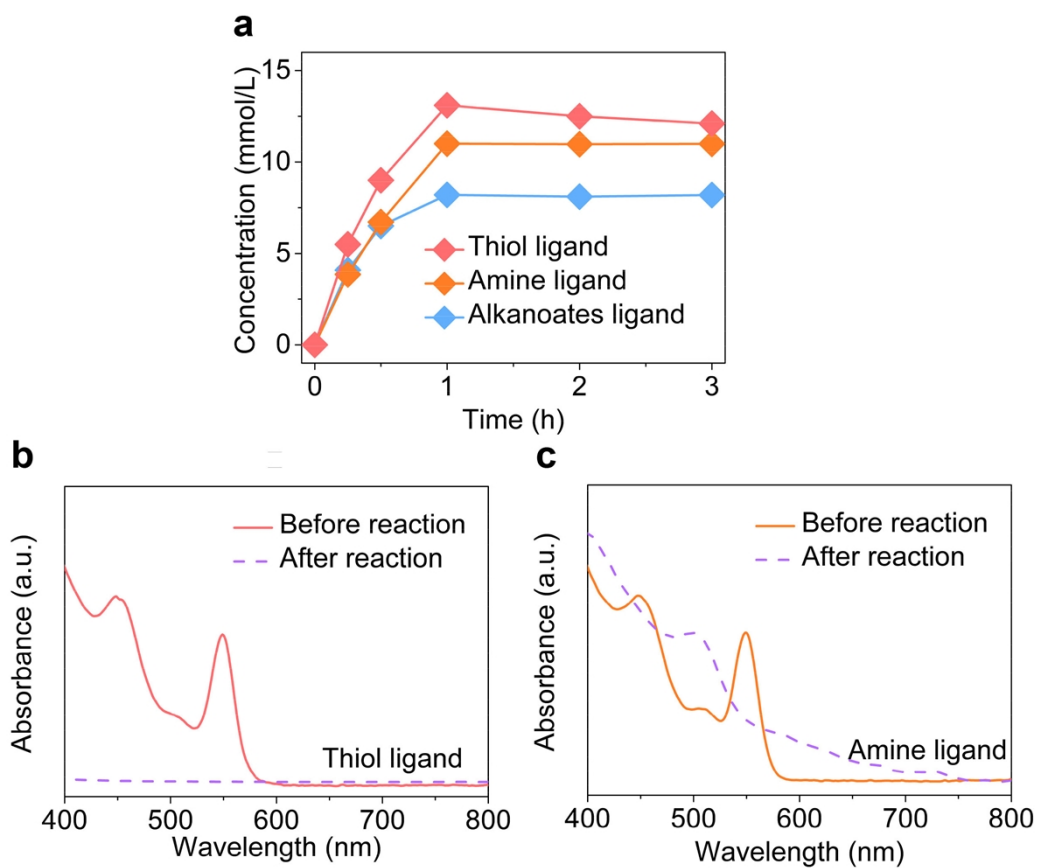


Fig S5. (a) Time courses of H₂O₂ production catalyzed by thiol-coated CdSe₅₅₀ QDs (pink), amine-coated CdSe₅₅₀ QDs (orange) and alkanates-coated CdSe₅₅₀ QDs (blue). (b) the UV-vis absorption spectra of the thiol-coated CdSe₅₅₀ QDs before reaction (solid line) and after reaction (dash line) (c) the UV-vis absorption spectra of the amine-coated CdSe₅₅₀ QDs before reaction (solid line) and after reaction (dash line).

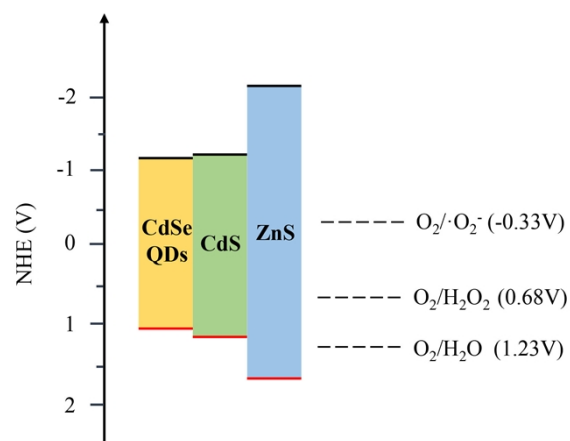


Fig S6. Energy levels of CdSe-based QDs and standard redox potential (*Versus* NHE) of oxygen reduction.

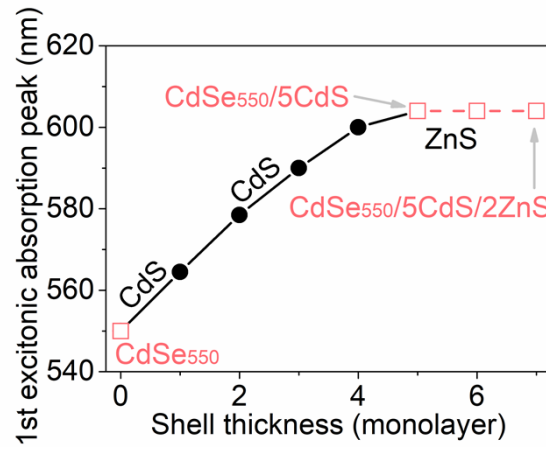


Fig. S7. Evolution of the 1st absorption peak of QDs with the shell thickness.

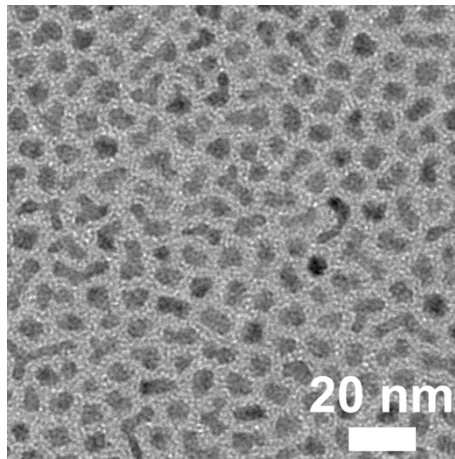


Fig S8. TEM images of CdSe₅₅₀/5CdS/3ZnS QDs.

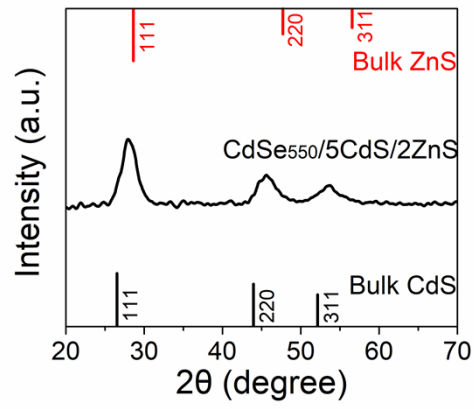


Fig S9. XRD pattern of CdSe₅₅₀/5CdS/2ZnS after reaction.

Before Reaction



After Reaction



Fig S10. The digital photographs of two-phase systems composed of an aqueous phase and an oil phase containing CdSe₅₅₀/5CdS/2ZnS before reaction (left) and after reaction (right).

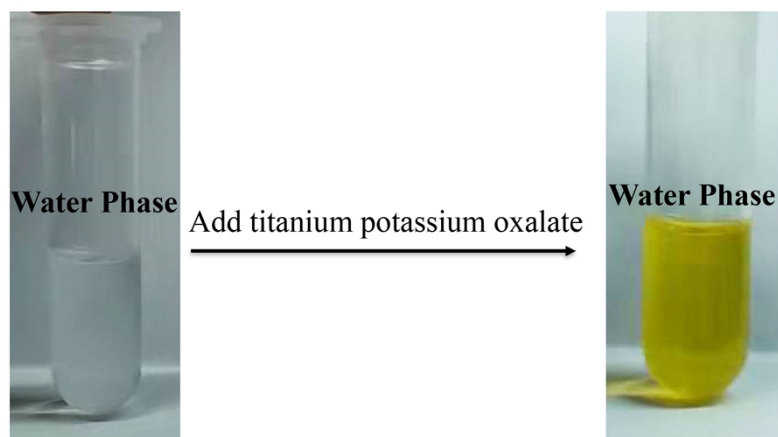


Fig S11. The digital photographs of the water phase in the two-phase system solution after photocatalytic reaction before (left) and after (right) adding titanium potassium oxalate.

Table S1. Summary of the photocatalytic H₂O₂ production with various photocatalysts.

Catalyst	Solvent	Concentration of photocatalyst /mg mL ⁻¹	Time/h	H ₂ O ₂ yields /mmol L ⁻¹	References
CdSe/5CdS/2ZnS	Oil/Water	~3.2	2	126	This work
a-C ₃ N ₄	Ethanol/water	1	4	~30	<i>J. Energy Chem. 2022</i> ¹
CdSe/KPN-HCP	Water	1	1	0.9	<i>Chem. Eng. J.2021</i> ²
Pd-BiVO ₄	CH ₃ OH/water	9.9	2	0.6	<i>Appl. Catal.2020</i> ³
MIL-125-NH ₂	benzyl alcohol /water	~0.7	3	~2.4	<i>Angew. Chem. Int. Ed. 2019</i> ⁴
SN-GQD/TiO ₂	2-propanol/water	0.5	1	0.45	<i>Appl. Catal.2018</i> ⁵
CdS-graphene	Water	1	12	~0.16	<i>J. Catal.2016</i> ⁶
g-C ₃ N ₄ /PDI _x	Water	1.7	48	1.7	<i>Angew. Chem. Int. Ed. 2014</i> ⁷
TiO ₂	benzyl alcohol /water	10	10	40	<i>ACS Catal. 2013</i> ⁸

Table S2. Simulation parameters used for ESR measurement (DMPO radical trapping agent).

Radicals	Simulation Parameters		
	A_N/G	A_H/G	Additional A_H/G
$\cdot O_2^-$	13.3	8.5	14.2
Ph \cdot CHOH	14.2	21.5	/

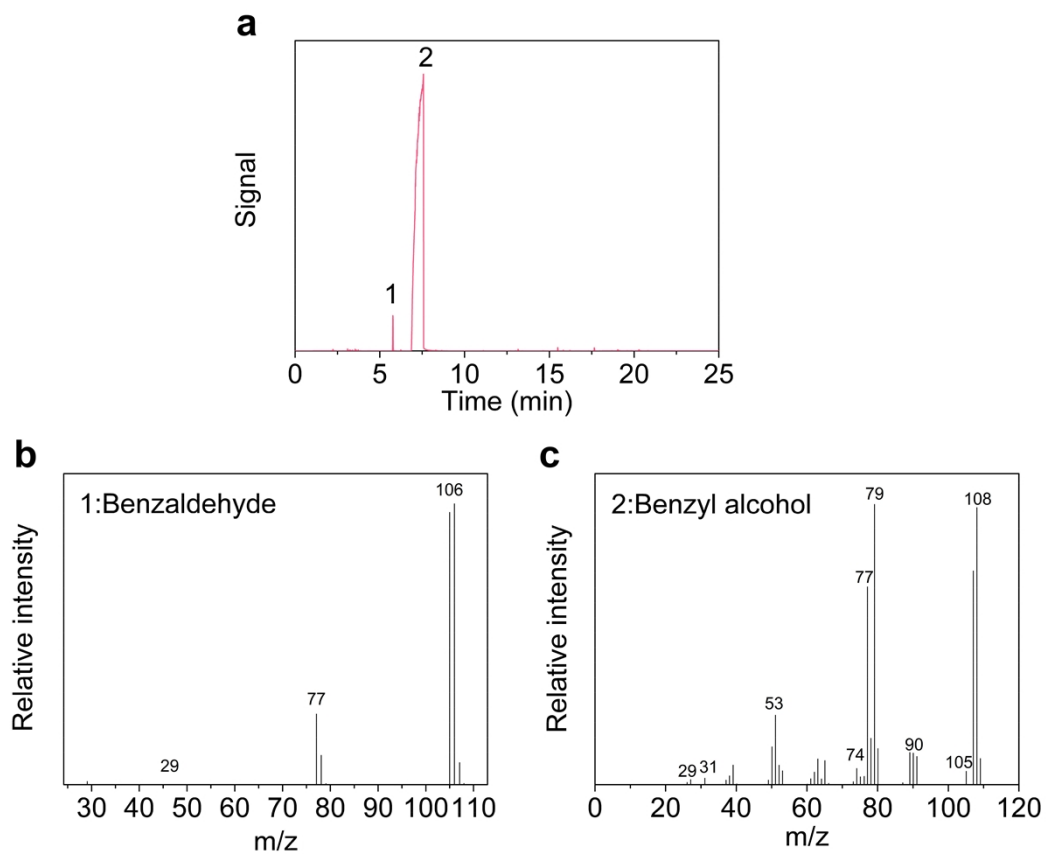


Fig S12. The oil phase product of the two-phase system catalyzed by CdSe₅₅₀/5CdS/2ZnS QDs. (a) GC spectral. (b)-(c) The MS spectral of the two peaks marked with 1, 2 in a. Benzyl alcohol was oxidized to benzaldehyde as product.

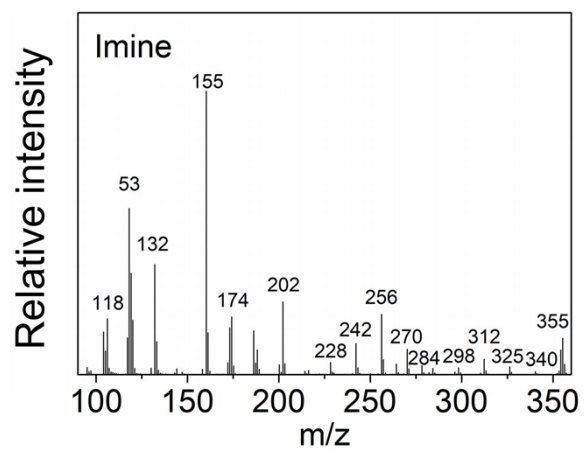


Fig S13. The MS spectral of the imine produced by the experiment.

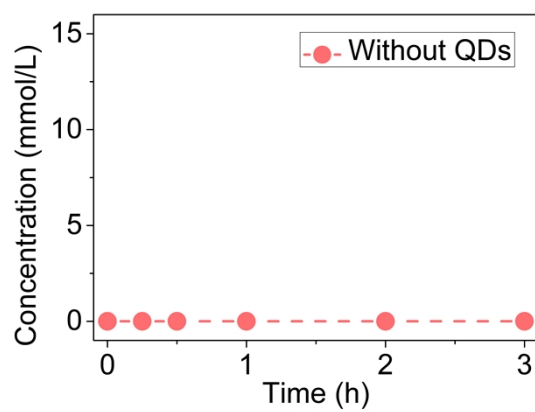


Fig S14. Time courses of H_2O_2 production of two-phase system without adding QDs.

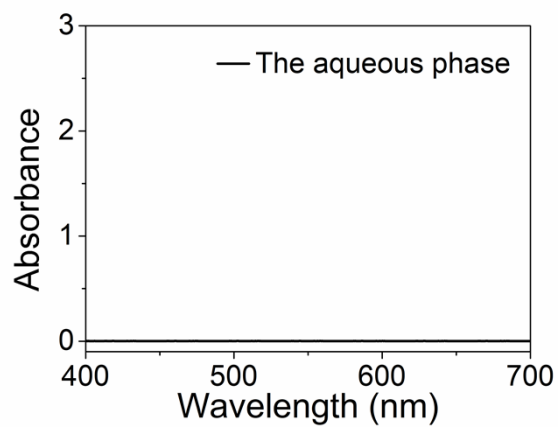


Fig S15. The UV-vis absorption spectra of the aqueous phase after reaction.

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