

Electronic Supplementary Information

Improving the Power Conversion Efficiency of Carbon Quantum Dot-Sensitized Solar Cells by Growing the Dots on a TiO₂ Photoanode In Situ

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1. Summary of the previous reported solar cells

Table S1. Key parameters of the solar cells sensitized by CQDs or GQDs reported in the literatures.^a

Type of the dot	Precursors and preparation method	Photoanode	Hybridization for CQDs ^b	J_{sc} (mA·cm ⁻²)	V_{oc} (V)	FF	PCE (%)	Ref.
CQDs	γ -butyrolactone, acid reflux	TiO ₂	physical adsorption	0.532	0.38	0.64	0.13	3
	CCl ₄ and NaNH ₂ , solvothermal	TiO ₂	hydrothermal ^c	0.69	0.46	0.43	0.13	4
	Chitosan-chitin, hydrothermal	ZnO (nanorods)	physical adsorption	0.674	9.265	0.43	0.077	5
	citric acid, urea, formic acid, microwave	TiO ₂	physical adsorption	0.99	0.49	0.50	0.24	6
	citric acid, ammonia, heating in the air	TiO ₂	physical adsorption (in acetone)	2.65	0.47	0.625	0.79	7
	citric acid, ethanediamine, hydrothermal	TiO ₂	<i>in situ</i> growth	6.47	0.43	0.31	0.87	This work
	citric acid, urea, microwave	TiO ₂	physical adsorption	only IPCE data were given				8
	graphite rods, electrochemical	TiO ₂ (nanotube)	physical adsorption (in acetone)	only EIS data were given				9
GQDs	Multi-step organic synthesis	TiO ₂	physical adsorption (in toluene/ethanol)	0.2	0.48	0.58	~0.06 ^d	10
	Multi-step organic synthesis	TiO ₂	<i>in situ</i> synthesis	2.49	0.55	0.64	0.87	11

^a When multiple solar cells appear in the same literature, parameters of the best cell are extracted. ^b If not stated, the physical adsorption occurs in aqueous solutions. ^c Hydrothermal treatment between TiO₂-coated photoanode and pre-synthesized CQDs.

^d Calculated values based on J_{sc} , V_{oc} , FF and AM 1.5 Global light.

2. Additional data

2.1 Result from ZnS passivation

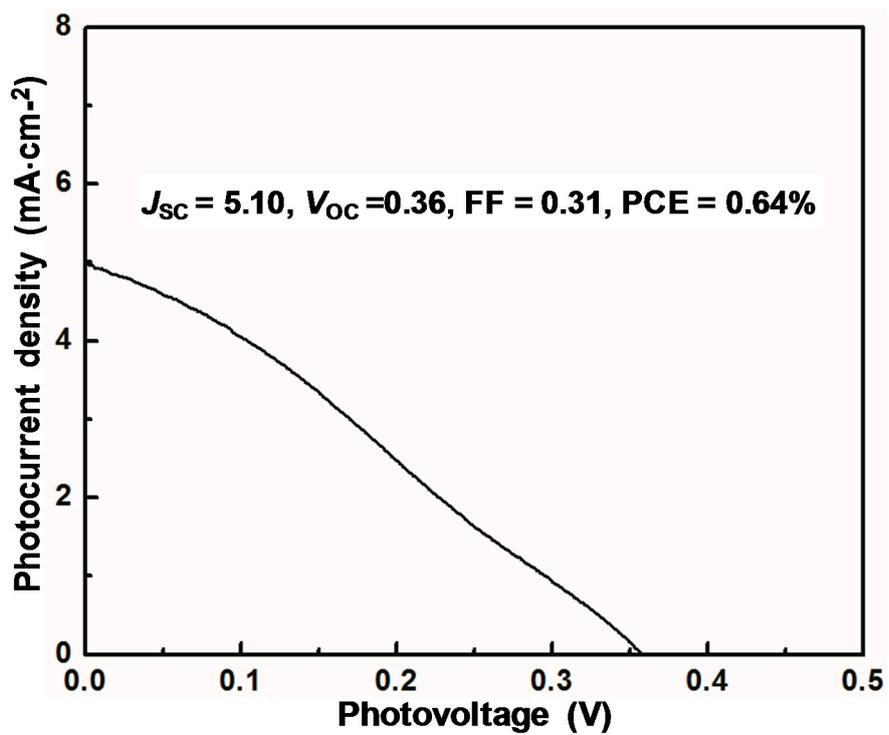


Figure S1. *JV* curve of the CQDSC constructed with the photoanode passivated by ZnS.

2.2 Results from post-annealing

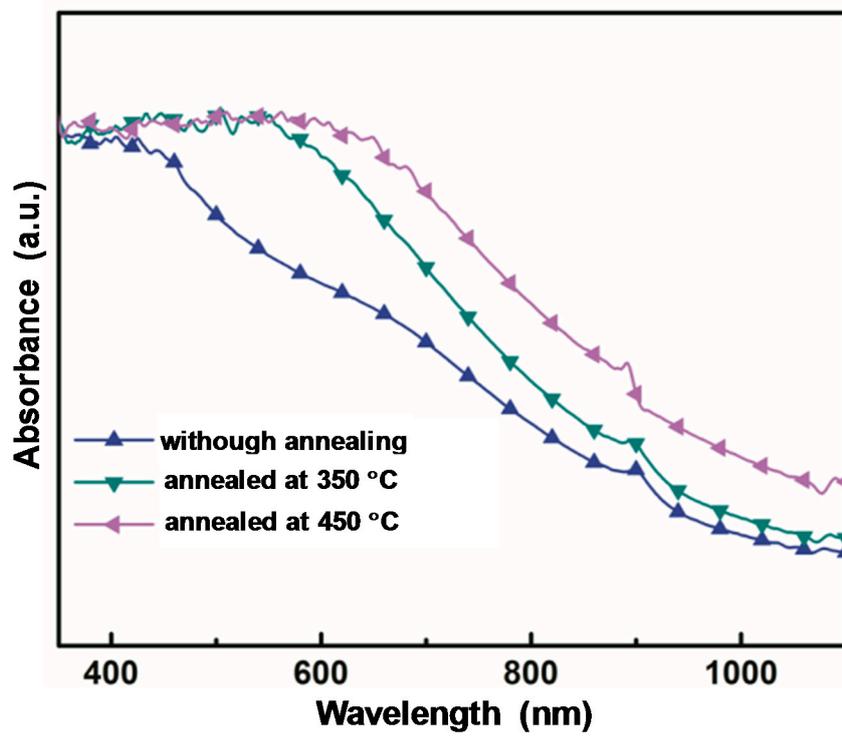


Figure S2. UV-vis-NIR absorption of CQDs-sensitized photoanodes without and with post-annealing at different temperatures.

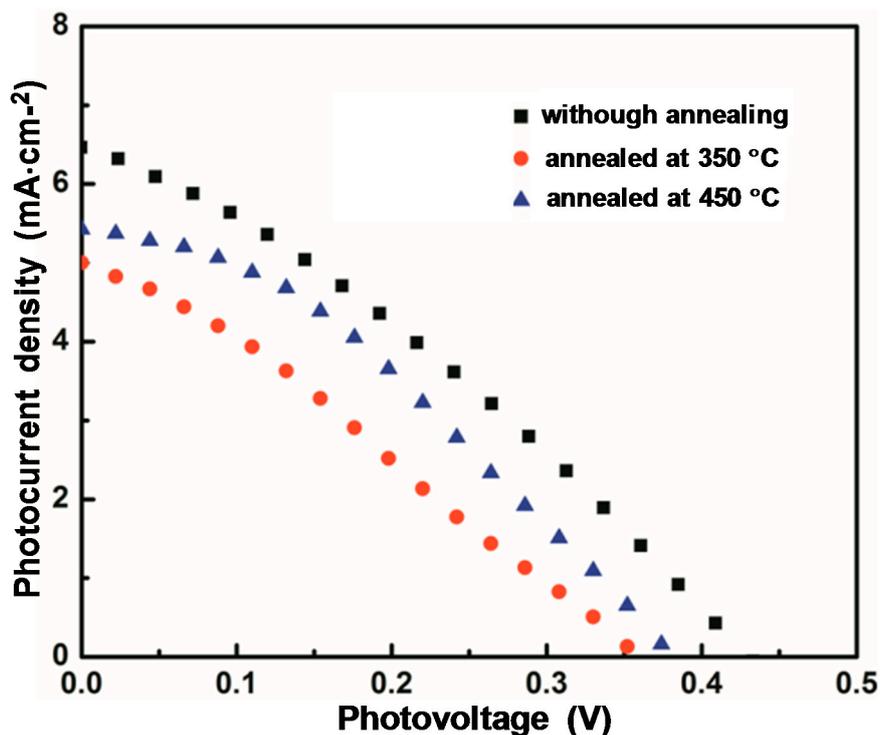


Fig. S3 *JV* characteristics of CQDSCs constructed by CQDs-sensitized photoanodes without and with post-annealing at different temperatures.

We speculate that during annealing, at least four effects will be induced. i) The peripheral organic functional groups of the CQDs will be destroyed, which will induce a more compact contact between CQDs and TiO₂ and might facilitate charge transfer. ii) As the annealing was performed in nitrogen, the carbon produced by the burning of the organic functional groups will (at least partially) remain on the TiO₂ surfaces, accounting for the increase of absorbance of the annealed photoanodes. iii) The originally hydrophilic surfaces of CQDs will become hydrophobic after annealing, which will cause a nonideal contact between the photoanode and the electrolyte and increase the resistance between them. iv) Finally, the annealing will disturb the surface states of the CQDs which are believed to govern the PL characteristics of the CQDs. The influence of the last factor on the performance of the solar cell is currently unknown, as the detailed origin of the PL properties of CQDs is quite complicated and is still under debate. The obtained experimental results of the influence of annealing on the performance of the CQDSC could be the integrated results of the above-mentioned effects.

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