

Supplementary Information of

Improving photovoltaic performance of solid-state ZnO/CdTe core-shell nanorod array solar cells by a thin CdS interfacial layer

Guanghui Zhang^a, Shenlong Jiang^b, Yue Lin^b, Wenzhen Ren^a, Hongbing Cai^b, Yukun Wu^a, Qun Zhang^{b,c}, Nan Pan^{b,c}, Yi Luo^{b,c} and Xiaoping Wang^{a,b,c*}

a, Department of Physics, University of Science and Technology of China, Hefei 230026, P. R. China

b, Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei 230026, P. R. China

c, Synergetic Innovation Center of Quantum Information & Quantum Physics, University of Science and Technology of China, Hefei, Anhui 230026, China

*Correspondence to Xiaoping Wang (xpwang@ustc.edu.cn)

In order to know whether the oxidation of CdTe occurs during the process of CdCl₂ treatment and annealing in air, we carried out the XPS measurement and observed the signal of Te oxide in the XPS spectra, as shown in Figure.S1.

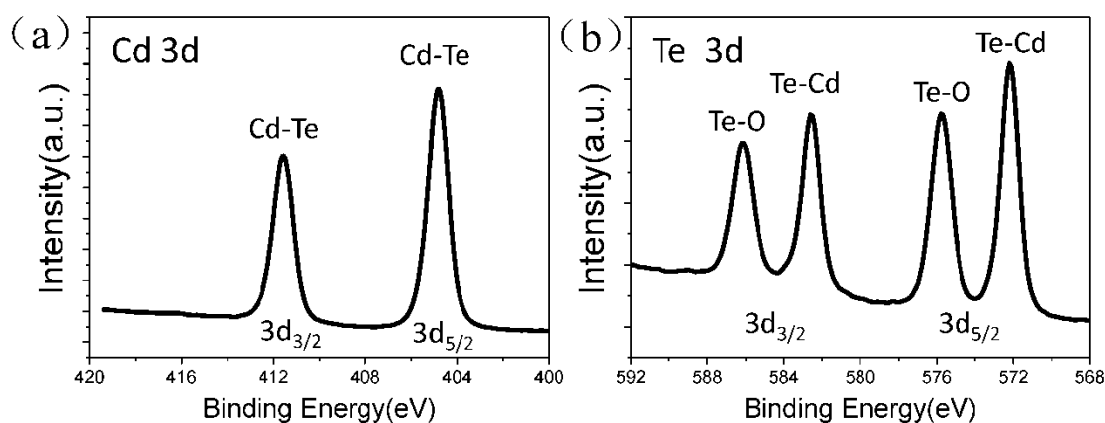


Figure S1. Cd 3d (a) and Te 3d (b) in XPS spectra of annealed ZnO/CdS/CdTe NR array.

Table S1. Summarized data of short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF), and overall power conversion efficiency (η) of ZnO/CdS/CdTe core-shell nanorod array solar cells with 0, 2, 4, 8 nm CdS interfacial layer.

CdS thickness	J_{sc} ($\text{mA}\cdot\text{cm}^{-2}$)	V_{oc} (mV)	FF (%)	η (%)
(0-nm CdS)	4.74 ± 0.59	165 ± 9	30.5 ± 0.66	0.24 ± 0.04
(2-nm CdS)	6.82 ± 0.26	203 ± 28	35.4 ± 1.01	0.49 ± 0.10
(4-nm CdS)	6.82 ± 0.30	306 ± 14	34.7 ± 1.97	0.72 ± 0.08
(8-nm CdS)	6.47 ± 0.35	312 ± 12	33.4 ± 0.75	0.67 ± 0.04

Table S2. The comparison of the performances for several previous reported one-dimensional ZnO (or TiO₂)/CdTe solar cell devices and ours.

Materials	Device architectures	J_p or J_{sc} ($\text{mA}\cdot\text{cm}^{-2}$)	V_{oc} (mV)	FF (%)	η (%)	Ref
ZnO NR/CdTe	Photoelectrochemical	5.9	N.A.	N.A.	N.A.	Ref 14
ZnO NR/CdSe/CdTe	Photoelectrochemical	14.3	N.A.	N.A.	N.A.	Ref 15
ZnO NR/CdTe/ZnS	Photoelectrochemical	13.8	N.A.	N.A.	N.A.	Ref 16
ZnO/CdTe NT	Photoelectrochemical	4.56	N.A.	N.A.	N.A.	Ref 17
ZnO NR/CdS/CdTe	Liquid-state	4.93	580	37	1.05	Ref 18
TiO ₂ NT/CdTe	Solid-state	1.23	230	30	~0.1	Ref 23
TiO ₂ NR/CdTe	Solid-state	0.67	650	17	0.07	Ref 24
ZnO NR /CdTe/CuSCN	Solid-state	0.19	120	29	0.007	Ref 25
ZnO NR/ CdS(4 nm)/CdTe	Solid-state	6.82	306	34.7	0.72	Ours

The impedance spectroscopy measurement was carried out with a two-electrode configuration (the FTO as working electrode and the Au electrode as both of the counter and the reference electrode^{1, 2}) in dark condition by applying a sinusoidal perturbation of 10 mV at -0.1V bias voltage with the frequencies changing from 100 kHz to 0.01 Hz. Figure S2a show the impedance spectra of ZnO/CdS/CdTe NRASC with 0, 2 and 4 nm thick CdS insert layer. The result of ZnO/CdS(8 nm)/CdTe is very similar to that of ZnO/CdS(4 nm)/CdTe. Figure S2 (b-d) are the enlarged impedance spectra of NRASCs at high frequency range. The inset of Figure S2a shows the schematic of equivalent circuit to fit the impedance spectra, where R_s and R_{sh} are the series and shunt resistance of NRASC, respectively. Based on the impedance spectra, R_s and R_{sh} can be estimated and the results are listed in Table S1. As seen, the series resistance for three NRASCs is kept about 250 Ω and show little dependent on the thickness of the CdS, implying that the inserted ultrathin CdS layer between ZnO core and CdTe shell will not contribute more resistance. Meanwhile, we find that the shunt resistance increases drastically after inserting CdS layer. The result indicates clearly that the CdS layer can passivate the surface of ZnO and consequently suppress the charge recombination at the interface as well as reduce the capture of electron by the defect traps, thereby improving the FF and J_{sc} of the NRASC (Figure 4c d in the manuscript).

Based on the diffusion-recombination model, we try to further estimate the carrier diffusion length L_n with the results of impedance spectra according to $L_n = l\sqrt{R_{sh} / R_s}$,^{2, 3} where l is the thickness of the NRASC and is about 450 nm in our case. The result is shown in Table S3. As seen, L_n is about several micrometers for our NRASCs, which is in agreement with the previous reported work by Jin et al.² Once again, we can observe the passivation effect of the CdS layer, i.e., after CdS coating, the carrier diffusion length can become twofold as compared to the sample without CdS layer.

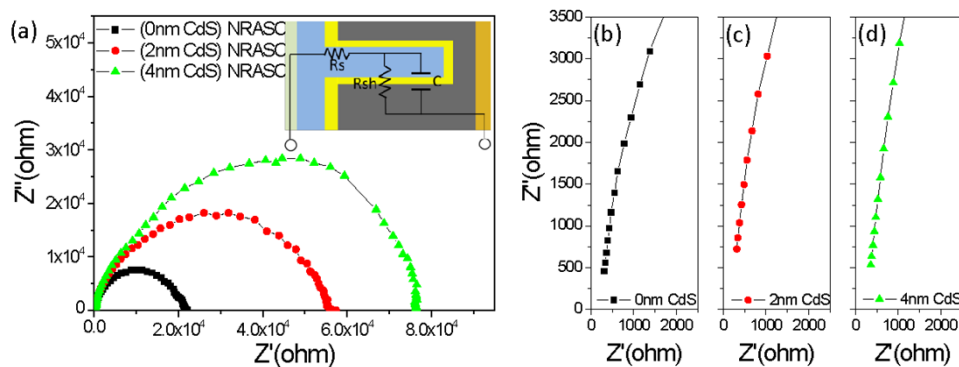


Figure S2. (a) Impedance spectra of ZnO/CdS/CdTe NRASC with the thickness of CdS varying from 0 to 4 nm. The inset shows the equivalent circuit for ZnO/CdS/CdTe core-shell NRASC. R_s , the series resistance; R_{sh} , shunt resistance; C , capacitance. (b), (c) and (d) are the enlarged

impedance spectra of NRASCs at high frequency range.

Table S3. Series resistance R_s , shunt resistance R_{sh} and capacitance C were extracted from impedance spectra. Carrier diffusion length L_n was estimated by R_s and R_{sh} .

CdS thickness	R_s (Ω)	R_{sh} (Ω)	C (nF)	L_n (μm)
(0-nm CdS) NRASC	260	22k	3.3	4.1
(2-nm CdS) NRASC	250	56k	3.5	6.7
(4-nm CdS) NRASC	250	76k	3.8	7.8

The power conversion efficiency of the devices can be further improved by increasing the ZnO nanorod length.

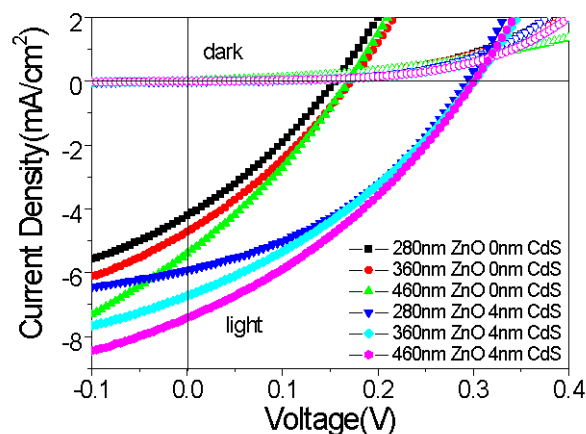


Figure S3. Typical J-V curves of ZnO/CdTe and ZnO/CdS (4 nm)/CdTe core-shell NRASCs with various ZnO NR lengths.

Table S4. Short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF) and power conversion efficiency (η) of core-shell NRASCs with various ZnO NR lengths.

	J_{sc} (mA/cm^2)	V_{oc} (mV)	FF (%)	η (%)
280 nm ZnO 0 nm CdS	4.20	155	30.4	0.20
360 nm ZnO 0 nm CdS	4.71	169	30.5	0.24
460 nm ZnO 0 nm CdS	5.39	170	29.7	0.27
280 nm ZnO 4 nm CdS	5.92	294	36.1	0.63
360 nm ZnO 4 nm CdS	6.71	300	33.5	0.67

Reference

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3. F. Fabregat-Santiago, G. Garcia-Belmonte, I. Mora-Sero and J. Bisquert, *Physical Chemistry Chemical Physics*, 2011, **13**, 9083-9118.