

Supporting Information

Chloride Treatments for High Efficient Aqueous- Processed CdTe Nanocrystal Based Hybrid Solar Cells

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Calculation of the texture coefficients and standard deviation. The texture coefficients, C_{hkl} , were calculated using Equation (1). And the standard deviation σ of the texture coefficients was calculated from Equation (2). I_{hkl} is the intensity of the reflection from plane(hkl), $I_{r,hkl}$ is the relative intensity of planes for the powder, n_p is the number of reflections shown in the diffractogram. The results were summarized in Table S3.

$$C_{hkl} = \frac{\frac{I_{hkl}}{I_{r,hkl}}}{1 / \left(\frac{1}{n_p} \sum_{n_p=1}^{n_p} \frac{I_{hkl}}{I_{r,hkl}} \right)} \quad (1)$$

$$\sigma = \sqrt{\sum 1/n_p (C_{hkl} - 1)^2} \quad (2)$$

Figure S1. Molecular structure of the conjugated polymer PFBTBr.

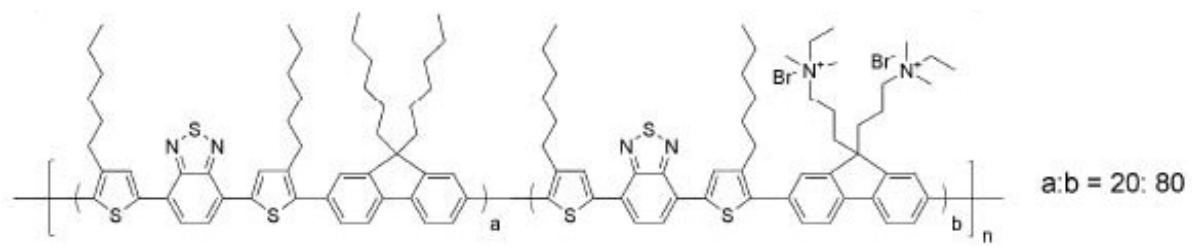


Figure S2. Optical micrographs and pictures of the CdTe films with CdCl₂ (a, d) spincoat, (b, e) dip and (c, f) drop treatment.

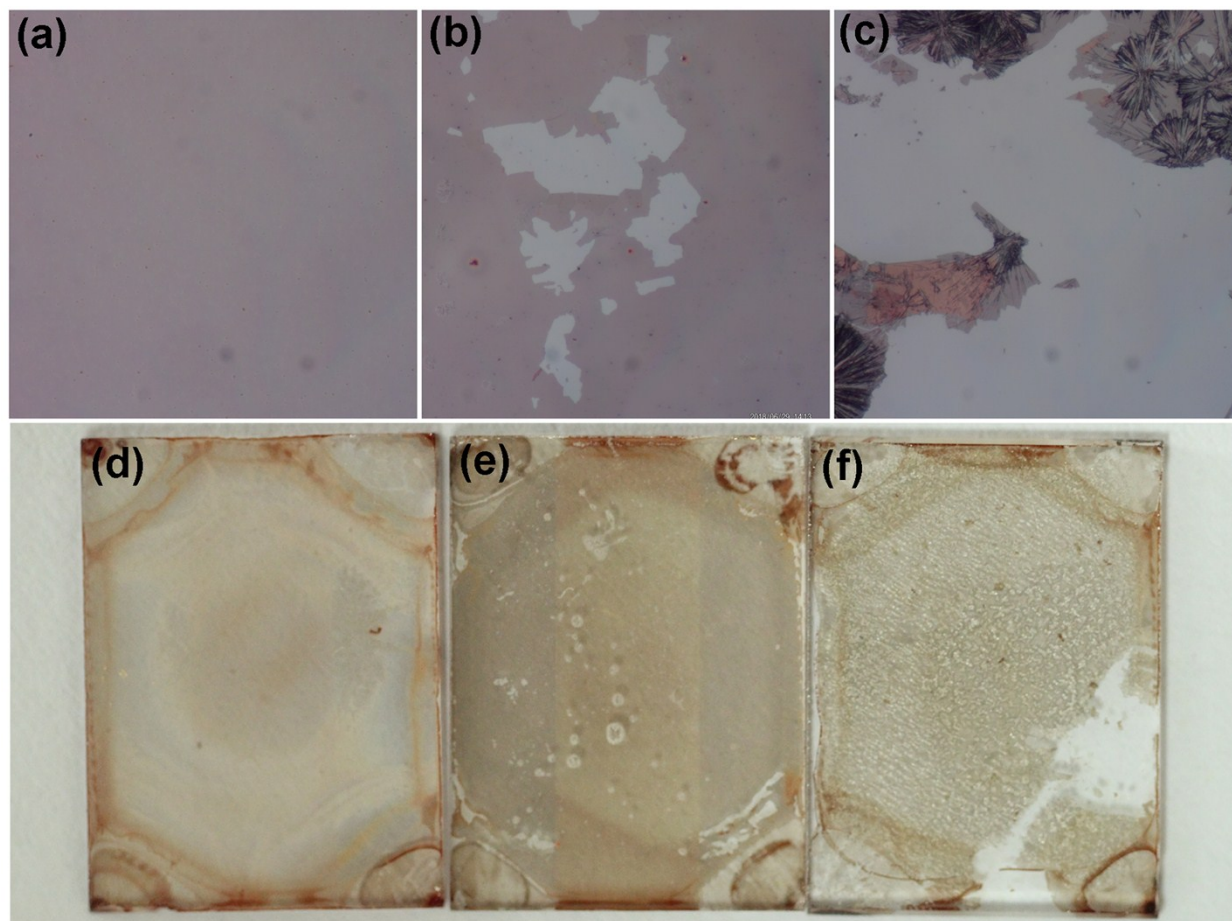


Figure S3. The histograms of the PCEs for the devices without (a) and with (c) CdCl_2 treatment.

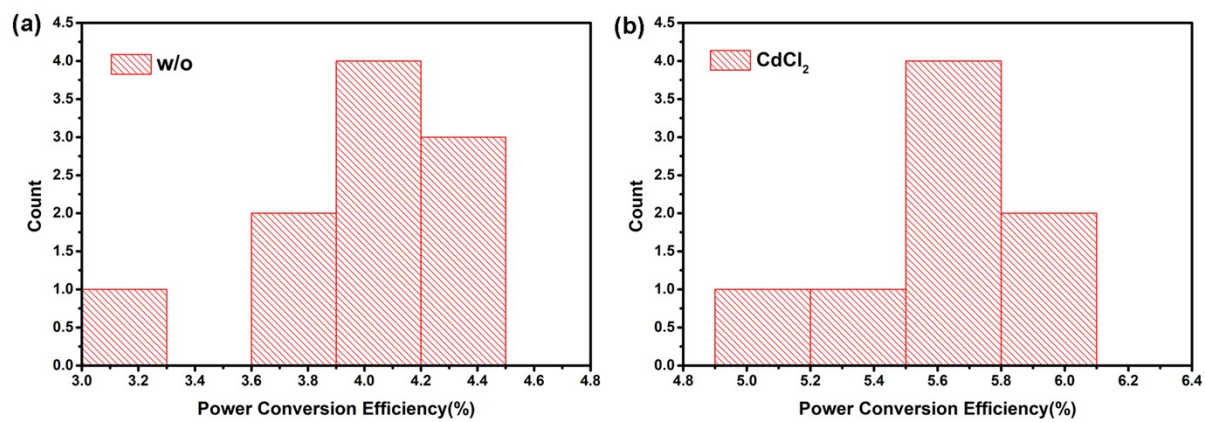


Figure S4. KPFM topology (left) and potential (right) images of the CdTe films without (a, b) and with (c, d) CdCl₂ treatment.

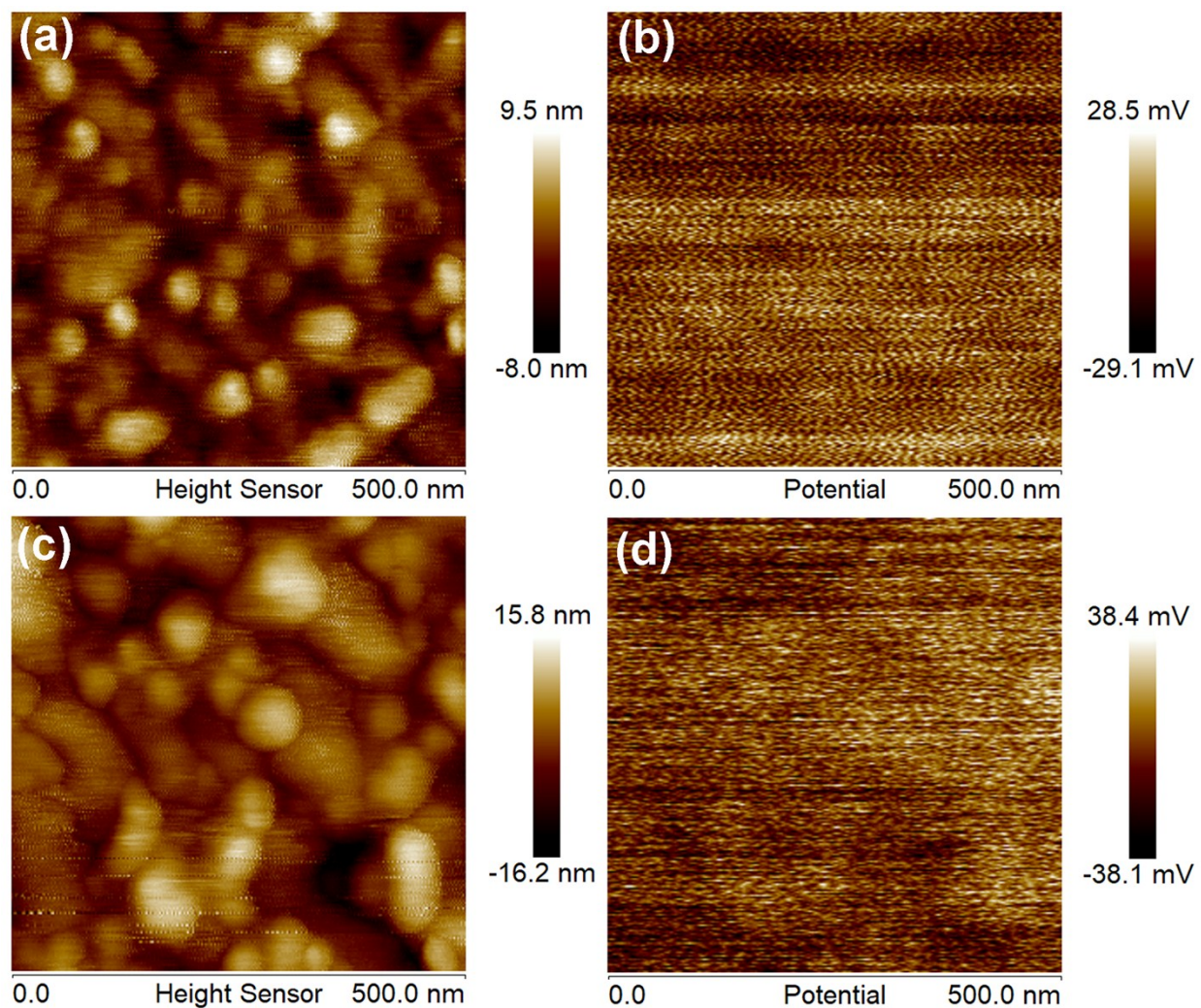


Figure S5. TG-DTG curves of PFBTBr.

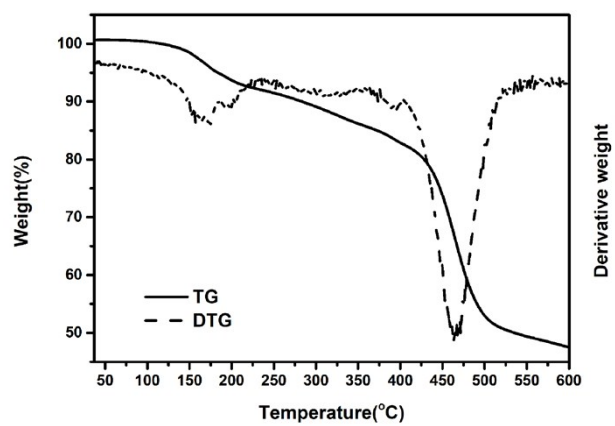


Table S1. Summary of the CdTe NCs based inorganic solar cells (ISCs), hybrid solar cells (HSCs) and quantum dot sensitized solar cells (QDSSCs) with literature reports.

Material	Device	PCE	Solvent	Ref.
CdTe NRs	ISCs	3.00	Pyridine	<i>Science</i> 2005, 310 , 462-465.
CdTe NCs	HSCs	0.421	Chloroform: pyridine	<i>Solar Energy Materials & Solar Cells</i> 2006, 90 , 1849–1858.
CdSe _x Te _{1-x} tetrapod	HSCs	1.13	Chloroform: pyridine	<i>Nanotechnology</i> 2006, 17 , 4041–4047
CdTe NPs	HSCs	0.06	Pyridine: chloroform	<i>Solar Energy Materials & Solar Cells</i> 2009, 93 , 1482–1487
CdSe/CdTe-tetrapod	HSCs	0.62	Pyridine: chloroform	<i>Adv. Mater.</i> 2009, 21 , 4461–4466
CdTe QDs	QDSSCs	2.20	Water	<i>Solar Energy Materials & Solar Cells</i> 2010, 94 , 2046–2051
CdTe NCs	HSCs	3.20	Chloroform: pyridine	<i>Adv. Mater.</i> 2011, 23 , 5451–5455
CdTe NCs	ISCs	6.90	Pyridine:1-propanol	<i>Nano Lett.</i> 2011, 11 , 2856–2864
CdTe/CdS QDs	HSCs	3.80	Water	<i>Chem. Sci.</i> 2011, 2 , 1396
CdTe NCs	HSCs	0.86	Water	<i>ACS Appl. Mater. Interfaces</i> 2011, 3 , 2919–2923
CdTe NCs	HSCs	2.14	Water	<i>Energy Environ. Sci.</i> 2011, 4 , 2831
CdTe NCs	ISCs	5.15	Pyridine:1-propanol	<i>J. Mater. Chem.</i> 2012, 22 , 19207
CdTe NCs	ISCs	12.3	Pyridine:1-propanol	<i>Nano Lett.</i> 2014, 14 , 670-675
CdSe/CdTe tetrapod	HSCs	3.30	Toluene	<i>Adv. Funct. Mater.</i> 2014, 24 , 1904–1910
CdTe NCs	ISCs	11.3	Pyridine	<i>ACS Nano</i> 2014, 8 , 9063-9072
CdTe/CdSe NCs	ISCs	5.81	Pyridine:1-propanol	<i>J. Mater. Chem. C</i> 2015, 3 , 4227--4234
CdTe NCs	ISCs	10.3	Pyridine	<i>J. Am. Chem. Soc.</i> 2016, 138 , 7464-7467
CdTe NCs	HSCs	3.61	Water	<i>Adv. Energy Mater.</i> 2013, 3 , 433–437
CdTe NCs	HSCs	3.30	Water	<i>Adv. Funct. Mater.</i> 2013, 23 , 4035–4042

CdS/CdTe NCs	ISCs	3.98	Water	<i>Adv. Energy Mater.</i> 2014, 4 , 1400235
CdTe NCs	HSCs	5.18	Water	<i>J. Mater. Chem. A</i> 2015, 3 , 10969–10975
CdTe NCs	HSCs	4.32	Water	<i>ACS Appl. Mater. Interfaces</i> 2015, 7 , 7146-7152
CdSe _x Te _{1-x} NCs	ISCs	3.35	Water	<i>ACS Appl. Mater. Interfaces</i> 2015, 7 , 23223-23230
CdTe/CdS NCs	ISCs	6.56	Water	<i>ACS Appl. Mater. Interfaces</i> 2016, 8 , 900-907
CdTe NCs	HSCs	4.32	Water	<i>ACS Appl. Mater. Interfaces</i> 2016, 8 , 7101-7110
CdTe NCs	HSCs	5.90	Water	<i>ACS Appl. Mater. Interfaces</i> 2017, 9 , 31345-31351
CdTe NCs	HSCs	6.36	Water	<i>Small</i> 2017, 13 , 1603771
CdTe NCs	HSCs	4.80	Water	<i>ACS Appl. Mater. Interfaces</i> 2017, 9 , 17942–17948

Table S2. Photovoltaic performances of the cells with CdCl₂ treatment applied in four different methods on the CdTe layer.

	V _{oc} (V)	J _{sc} (mAcm ⁻²)	FF(%)	PCE(%)
w/o	0.620	16.34	44.29	4.49
Spincoat	0.638	20.76	45.34	6.01
Dip	0.606	18.00	41.29	4.50
Drop	0.587	9.65	31.60	1.78
Vapour	0.610	19.66	43.12	5.17

Table S3. Photovoltaic performances of the cells with CdCl₂ treatment applied on the CdTe and CdTe:PFBTBr layers through spincoat method.

	V _{oc} (V)	J _{sc} (mAcm ⁻²)	FF(%)	PCE(%)
w/o	0.620	16.34	44.29	4.49
CdTe	0.638	20.76	45.34	6.01
CdTe:PFBTBr	0.616	19.24	32.73	3.88

Table S4. Texture coefficients and the standard deviation of the cells without and with CdCl₂ treatment.

	C ₁₁₁	C ₂₂₀	C ₃₁₁	σ
w/o	1.28	0.88	0.84	0.20
CdCl ₂	1.88	0.53	0.74	0.53