Supplementary Materials

$PbS_{1-x}Se_x$-Quantum-Dot@MWCNT/P3HT Nanocomposites with Tunable Photoelectric Conversion Performance

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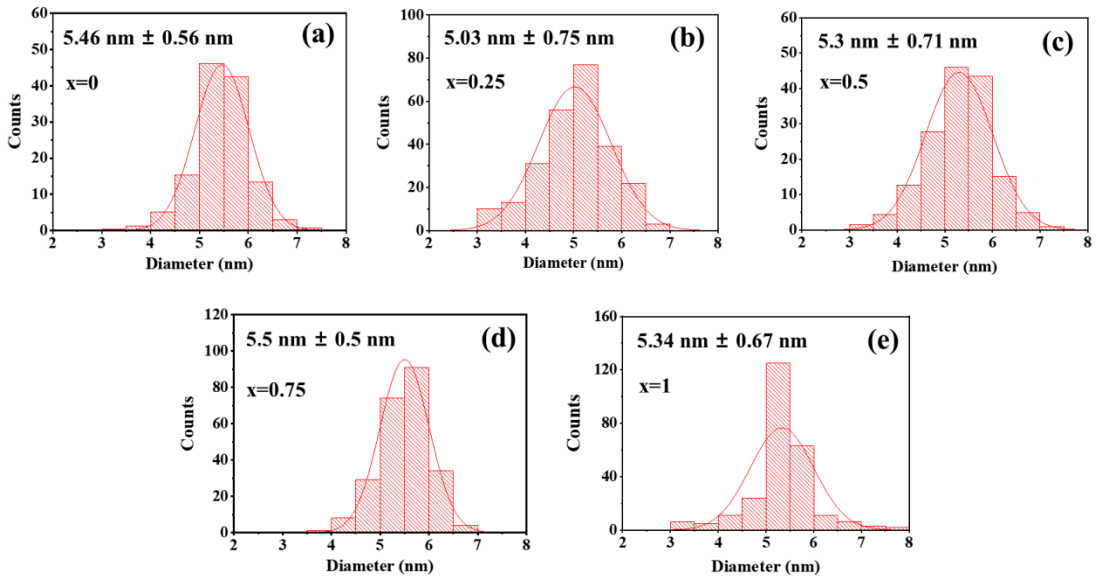

Figure S1. Histogram of size distribution of $PbS_{1-x}Se_x$ (x = 0, 0.25, 0.5, 0.75, 1) QDs.

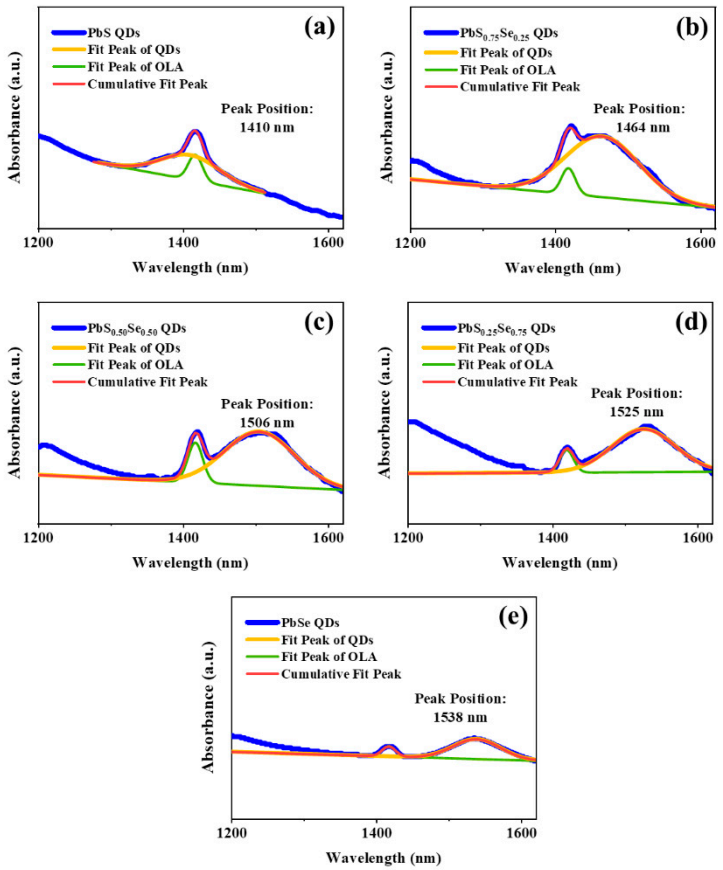

Figure S2. Fitted absorption spectra of $PbS_{1-x}Se_x$ (x = 0, 0.25, 0.5, 0.75, 1) QDs. The ligand OLA on the QDs surface could produce many tiny peaks in the absorption spectra, only the most conspicuous one at 1418 nm was taken into consideration for the Gaussian fitting to obtain the location of the first excitation peaks of the QDs.

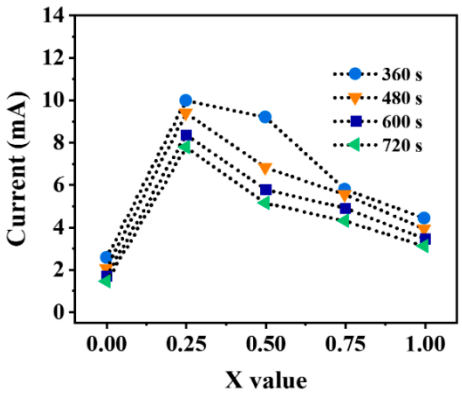

Figure S3. Photocurrents measured at different times as a function of x value in $PbS_{1-x}Se_x$-QD@MWCNT/P3HT.

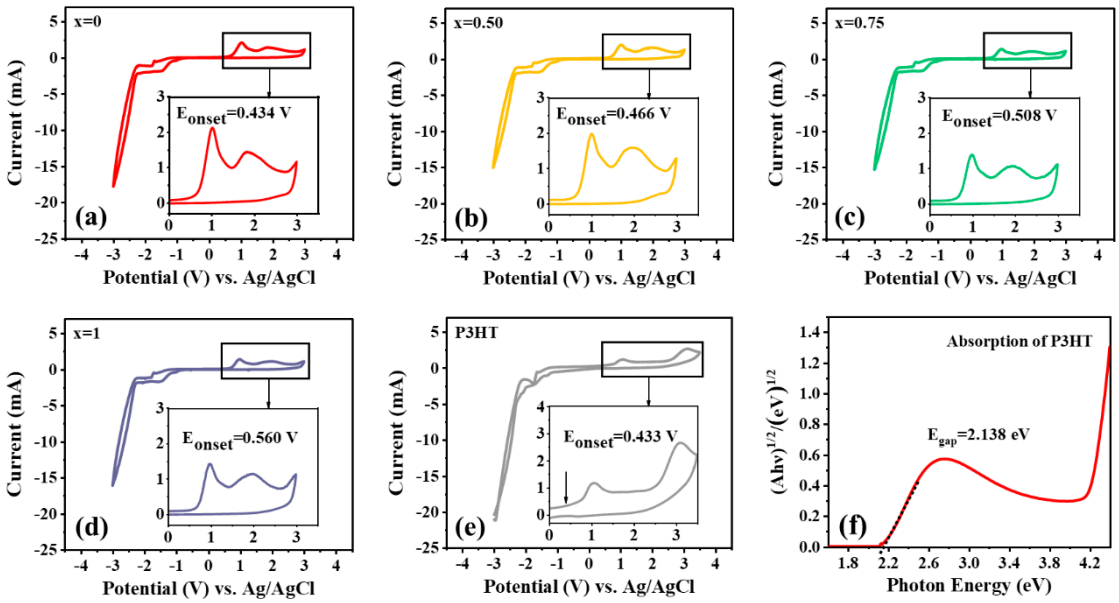

Figure S4. (a)-(e) Cyclic voltammetry (CV) curves of PbS, $PbS_{0.50}Se_{0.50}$, $PbS_{0.25}Se_{0.75}$, PbSe QDs and P3HT measured in 3.5M KCl at room temperature. E_{onset} is the initial position of the oxidation peak, and $E_{HOMO} = -(E_{onset} + \Delta E_{Ag/AgCl}) - 4.5$, where $\Delta E_{Ag/AgCl} = 0.204$ (V). **(f)** Absorption spectrum of P3HT.

Table S1. Energy level alignment of P3HT and $PbS_{1-x}Se_x$ (x = 0, 0.25, 0.5, 0.75, 1) QDs

Samples	E_{onset} (V)	HOMO (eV)	E_g (eV)	LUMO (eV)
P3HT	0.433	-5.137	2.138	-2.999
PbS	0.434	-5.138	0.879	-4.259
$PbS_{0.75}Se_{0.25}$	0.444	-5.148	0.847	-4.301
$PbS_{0.50}Se_{0.50}$	0.466	-5.17	0.823	-4.347
$PbS_{0.25}Se_{0.75}$	0.508	-5.212	0.813	-4.399
PbSe	0.560	-5.264	0.806	-4.458

*E_{onset} was obtained from CV tests; HOMO was calculated from $E_{HOMO} = -(E_{onset} + \Delta E_{Ag/AgCl}) - 4.5$. E_g represented the band gap according to the absorption spectrum and the LUMO was obtained from HOMO and E_g.

Synthesis of $PbS_{1-x}Se_x$ (x = 0, 0.25, 0.5, 0.75, 1) QDs [1–3]

20 mL of S-OLA, 20 mL of Se-OLA and 5 mL of $PbCl_2$-OLA precursors were prepared in advance as described in the experimental section. Following the synthesis procedure of $PbS_{0.75}Se_{0.25}$ QDs, the synthesis parameters for PbS, $PbS_{0.50}Se_{0.50}$, $PbS_{0.25}Se_{0.75}$ and PbSe QDs are shown in Table S2.

Table S2. Synthesis parameters of $PbS_{1-x}Se_x$ (x = 0, 0.25, 0.5, 0.75, 1) QDs.

Sample	Volume of $PbCl_2$-OLA (mL)	Volume of S-OLA (mL)	Volume of Se-OLA (mL)	Temperature of $PbCl_2$-OLA (℃)	Temperature of (S+Se)-OLA (℃)	Time (s)
PbS	5	1.7	0	90	90	300
$PbS_{0.75}Se_{0.25}$	5	3.8	1.2	95	150	40
$PbS_{0.50}Se_{0.50}$	5	2.5	2.5	100	150	60
$PbS_{0.25}Se_{0.75}$	5	1.2	3.8	105	150	100
PbSe	5	0	1.7	120	240	300

Table S3. Atomic ratio of S/Se in $PbS_{1-x}Se_x$ (x = 0.25, 0.5, 0.75) QDs measured by XPS

Samples	Atomic ratio of S/Se
$PbS_{0.75}Se_{0.25}$	3.13
$PbS_{0.5}Se_{0.5}$	1.08
$PbS_{0.25}Se_{0.75}$	0.34

References

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