Quantum Junction Solar Cells
Supplementary Information

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S1. Details of self-consistent optoelectronic simulations

V_{MPP}, J_{sc} and *PCE* were simulated using a combination of SCAPS and Sentaurus. Results were found to be consistent between the simulators under identical materials conditions.

DH Architecture

Parameters	**N-TiO2**	**p-PbS**
Band gap	3.2 eV	Variable (0.6-1.6 eV)
Electron affinity	4.1 eV	Variable [1]
Mobility	1 cm^2/Vs	$5x10^{-3}$ cm^2/Vs
Lifetime	10 us	1 us
Thickness	0.5 um	0.4 um
Doping	10^{16} cm^{-3}	10^{16} cm^{-3}

QJ Architecture

Parameters	**n-PbS**	**p-PbS**
Band gap	Variable (0.6-1.6 eV)	Variable (0.6-1.6 eV)
Electron affinity	Variable[1]	Variable[1]
Mobility	$1x10^{-2}$ cm^2/Vs	$1x10^{-4}$ cm^2/Vs
Lifetime	1 us	1 us
Thickness	0.4 um	0.05 um
Doping	10^{16} cm^{-3}	$5x10^{18}$ cm^{-3}

The spectrum of absorption coefficients used in the model was chosen agree with experimentally-measured quantum dot film absorbance.

S2. TMAOH-treated p-type PbS film

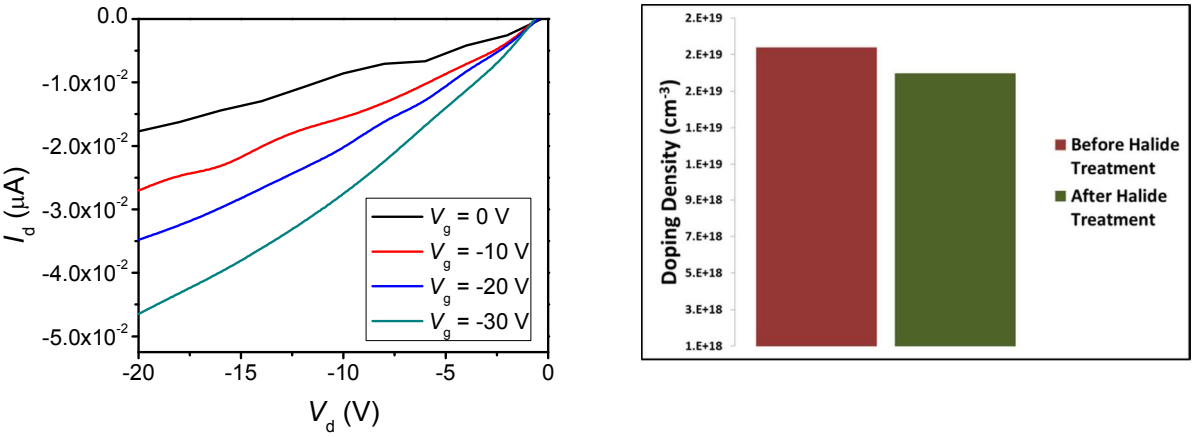

Fig S2. (a) FET response of a film created with TMAOH treatment in ambient atmosphere, clearly showing p-type behaviour (W=1 mm, L=5 um); and **(b)** The p-type doping density of TMAOH treated film after soaking in methanol solution for 10min. The doping density remains virtually unchanged suggestive of robust p-type doping by the TMAOH treatment.

Sample	Doping Density (cm^{-3})
1	2.20E+19
2	1.00E+19
3	1.50E+19
4	2.30E+19
5	1.90E+19
6	2.10E+19
Standard Deviation	**4.96655E+18**

Table S2. FET samples of p-type CQD films made using the TMAOH treatment. Results show a reproducible doping density around 10^{19} cm^{-3}.

S3. Capacitance-V Calculation

The Schottky plot (C^{-2} vs. V) is used to estimate the carrier density of the n-type PbS CQDs based on a p+-n approximation. The doping density (N_D) was calculated using the slope of plot.

$$\frac{1}{C^2} = -\frac{2\ V}{A^2 \varepsilon_0 \varepsilon_r q N_D}$$

C = capacitance of the space charge region (depletion region)
ε_0 = permittivity of free space
ε_r = dielectric constant of the PbS CQDs (=43)
N_D = donor density
A = area
V = applied potential
V_{bi} = built-in voltage (flat band potential)

S4. Junction Characterization.

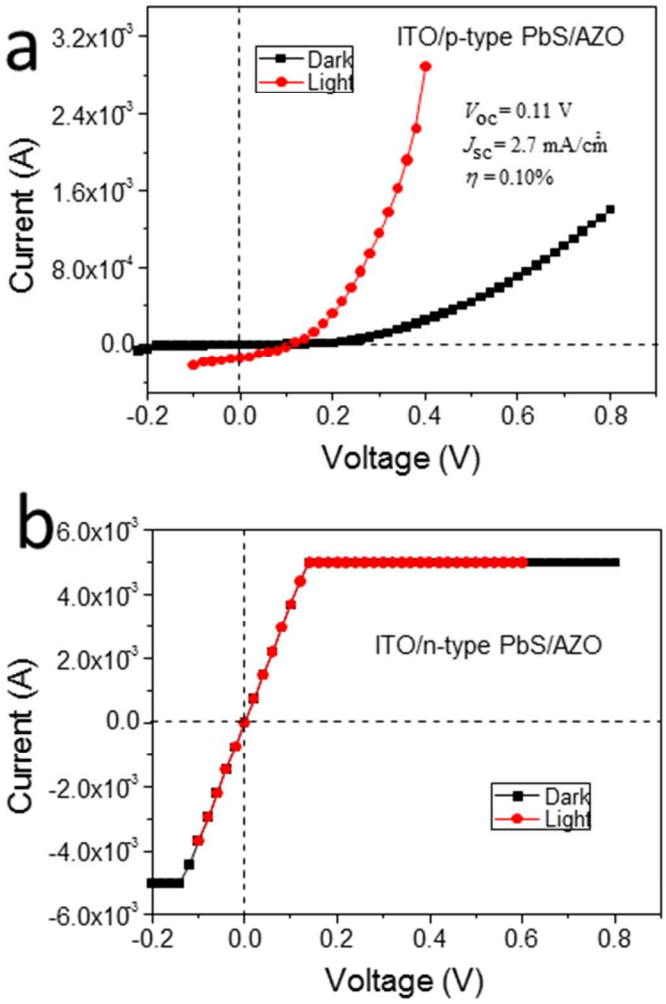

Fig S4. (a) Junction made only using the p-layer showing very weak rectification and negligible photovoltaic performance and **(b)** Junction made only using the n-layer showing no rectification. The plateaus at positive and negative biases are due to a current compliance of 5 mA set on the instrument.

S5. Calculation of Voc limit

From the C. H. Henry paper "Limiting efficiencies of ideal single and multiple energy gap terrestrial solar cells" (J. Appl. Phys. 1980, 51, 4494):

$$V_{OC} = \frac{E_g}{q} - \frac{kT}{q}\ln(\frac{A}{qn_{ph}})$$

$$A \cong 5693 E_g^2 \frac{S}{cm^2}$$

$$n_{ph}(E_g) = \int_{E_g}^{\infty} \frac{dn_{ph}}{d\hbar\omega} d\hbar\omega$$

where E_g is the band gap, k is Boltzmann constant, T is temperature, q is elementary charge, A is E_g dependent parameter, n_{ph} is the sum of absorbed incident photon, S is the cell area, $\hbar\omega$ is the photon energy. For the QJSC using 0.6 eV PbS CQDs, the n_{ph} is integrated as 3.56×10^{17} $cm^{-2}sec^{-1}$ using the ASTMG173 solar spectrum spreadsheet, A is 2049.5 using $S = 1cm^2$, and the calculated maximum V_{oc} is 0.33 V. Experimentally, we obtained a maximum V_{oc} of 0.29, equal to about 80% of the theoretical limit.

S6. Absorbance of p and n-type layers

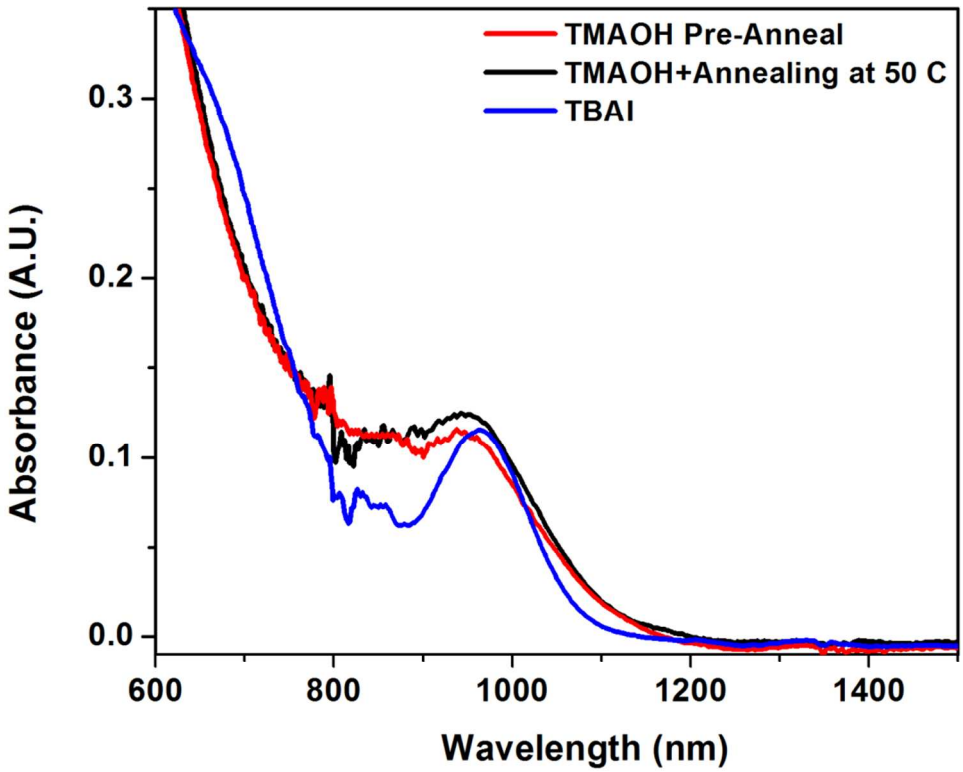

Figure S6. Absorbance of the p (TMAOH) and n-type (TBAI) layers showing quantum confinement is retained. Samples were made to have equal thickness of about 250 nm. TMAOH after the annealing step also retains quantum confinement. The excitonic peaks of both materials remain in the same position.