Unity Quantum yield of Charge Carrier Photogeneration and Band-Like Transport in Quantum-Dot Solids

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SUPPLEMENTARY INFORMATION

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1. SEM and TEM images of LbL deposited films

To evaluate the homogeneity of the PbSe QD films after deposition and to investigate whether sintering of particles occurred during the film preparation scanning electron microscopy (SEM) and high-resolution transmission electron microscopy (HR-TEM) were used. SEM was performed on QD films deposited on indium doped tin oxide (ITO) substrates using the same Layer-by-Layer procedure that was used in the terahertz, transient absorption and time-resolved microwave conductivity experiments. Ten deposition cycles were applied and 1,2-ethanediamine was used as substitute capping ligand. Images were obtained with a JEOL JSM-7500F Field emission SEM in secondary electron image mode at 5 kV. HR-TEM images were acquired with an aberration-corrected cubed Titan microscope operating at 300 kV. In this case PbSe QD films were deposited onto 15 nm thick SiN membranes using condition identical to those used to deposit the films that were used in the photoconductivity studies. To produce films that are sufficiently thin for TEM analysis only a single cycle of the LbL procedure was used.

Figure S1 shows SEM images at different magnifications. As can be seen in the top left image the film is smooth and homogeneous over tens of micrometers. Several very small pinholes are visible at higher magnification (top right image). Such pinholes will not influence the measurements reported here but would be detrimental for solar cells as they could cause shunting. In the bottom images the individual quantum dots can be recognized. It is clear that large cluster or wires are not formed.
Figure S1 SEM images at different magnifications of a PbSe QD films grown using the layer-by-layer technique.

Figure S2 shows a collection of high resolution TEM images of several films, while Figure S3 shows a high resolution zoom-in on a small part of a film. The TEM images clearly confirm that the QDs do not fuse together into large clusters or wires. On a very local scale it is hard to distinguish where one QD ends and the next one begins. One has to consider that the length of a 1,2-ethanediamine molecule is 4 Å, while the lattice constant of PbSe is 6 Å, which means that the separation between adjacent Pb and Se atoms is 3 Å. Hence, two QDs that are separated by the distance of a single 1,2-ethanediamine molecule will appear virtually continuous. However, close inspection of Fig. S3 shows clearly that the lattice planes of different QDs are different. If the QDs would sinter they would have a strong tendency to align their lattice planes, as this lowers the total free energy of the crystal. The polycrystallinity and the fact that the nanocrystals retain their spherical shape are clear indications that no significant sintering has occurred during the layer-by-layer deposition process.
Figure S2 Collection of TEM images of PbSe QD films grown using the layer-by-layer technique.
Figure S3 High resolution TEM image of a PbSe QD films grown using the layer-by-layer technique.
2. THz and TA transient at different intensities

Figure S4 shows a comparison of interband absorption transients with the real and imaginary THz conductivity transients of the same sample, at two different excitation densities. It is clear from the figure that the decay kinetics of the transient absorption signal and the real and imaginary THz conductivity are identical at both excitation densities.

Figure S4 Comparison of interband absorption transients (red curve, left axis) and the real and imaginary terahertz conductivity transients (black and green curves, respectively, right axis) at two different excitation densities of 0.15 absorbed photons per QD (a) and 0.23 absorbed photons per QD (b)
3. Temperature dependent decay kinetics

The decay of the photoconductivity signal depends strongly on temperature. Figure S5a shows undeconvoluted TRMC transients of $\Phi \Sigma \mu$ at an excitation density of 0.17 absorbed photons per QD and at different temperatures. Clearly the decay becomes faster as the temperature increases. Figure S5b shows the measured lifetimes $\tau_{1/2}$ (the time at which the photoconductivity is half of the maximum value) of the deconvoluted transients at low (black squares, 0.001 absorbed photons per QD) and high (red circles, 2 absorbed photons per QD) photoexcitation density.

At low excitation density higher order recombination is absent and the first order lifetime is obtained. The first order charge carrier lifetime is always longer than the laser pulse duration; at the lowest temperature it is three orders of magnitude longer. The decay rate is, hence, thermally activated. An Arrhenius fit to the first order decay results in an activation energy of $67 \pm 7$ meV. The higher order decay time (red circles in Fig. S5b) is always shorter than the experimental time resolution.

Figure S5 a) Photoconductivity transients at various temperatures for a fixed excitation density of 0.17 absorbed photons per QD. b) Charge carrier lifetime $\tau_{1/2}$ as a function of temperature at excitation densities of 0.001 (black squares) and 2 (red circles) absorbed photons per QD.

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4. Influence of recombination during the laser pulse on the measurement of the photogeneration yield and mobility of charge carriers

The total number of charges generated in the sample during the laser pulse is $\eta N_{\text{abs}}$, where $\eta$ is the quantum yield of charge carrier photogeneration and $N_{\text{abs}}$ is the number of absorbed photons per pulse. The rate of generation of charges is $\eta N_{\text{abs}}/\tau_{\text{las}}$, where $\tau_{\text{las}}$ is the laser pulse duration (i.e. the width of the laser pulse if approximated by a rectangular pulse). For first order recombination with rate constant $k_1$ the rate equation is

$$\frac{dN(t)}{dt} = \frac{\eta N_{\text{abs}}}{\tau_{\text{laser}}} - k_1 N(t)$$

(1)

$N(t)$ is the density of charge carriers present at time $t$. For a sufficiently long laser pulse equilibrium between generation and decay of charges is reached during the pulse, resulting in a maximum density of charge carriers $N_{\text{max}}$:

$$0 = \frac{\eta N_{\text{abs}}}{\tau_{\text{laser}}} - k_1 N_{\text{max}}$$

(2)

Or:

$$N_{\text{max}} = \frac{\eta N_{\text{abs}}}{k_1 \tau_{\text{laser}}}$$

(3)

This shows that the maximum number of charges, and hence the maximum in the photoconductance depends on the rate constant $k_1$. Since $k_1$ may depend on temperature (in fact it does strongly increase with increasing temperature) this may affect the measured value of $\Phi_{\text{max}} \sum \mu = (N_{\text{max}}/N_{\text{abs}}) \sum \mu$. In particular, an increase of $k_1$ may compensate an increase in $\Sigma \mu$.

The above is however only valid if the lifetime of the charge carrier ($\tau_1 = 1/k_1$) is equal to or smaller than $\tau_{\text{las}}$. For longer charge lifetimes the equilibrium is reached at the end of the laser pulse and $N_{\text{max}} = \eta N_{\text{abs}}$.

As discussed above (Figure S4) the first order charge lifetime is always longer than the laser pulse duration; at the lowest temperature it is three orders of magnitude longer. This is corroborated by fs resolved transient absorption measurements shown in Figure 1a of the manuscript that show a sustained optical bleach of the band edge exciton transition with no significant decay over the first ns after excitation. These results show that first order recombination does not play a significant role in the measured values of $\Phi_{\text{max}} \sum \mu$ and that the temperature dependence of $k_1$ cannot cause $\Phi_{\text{max}} \sum \mu$ to be constant.

At high excitation densities, there is significant second-order recombination during the laser pulse with a rate constant $k_2$.

The rate equation is:

$$\frac{dN(t)}{dt} = \frac{\eta N_{\text{abs}}}{\tau_{\text{laser}}} - k_2 N^2(t)$$

(4)
and the maximum density of charge carriers becomes:

\[ N_{\text{max}} = \sqrt{\frac{\eta N_{\text{abs}}}{\tau_{\text{laser}} k_2}} \]  

(5)

The second-order charge recombination rate is:

\[ k_2 = \frac{e \Sigma \mu}{\varepsilon_0 \varepsilon} \]  

(6)

where \( \varepsilon_0 \) is the vacuum permittivity, \( \varepsilon \) is the relative dielectric of the material and \( \Sigma \mu \) is the sum of the electron and hole mobility. We obtain:

\[ \Phi_{\text{max}} \Sigma \mu = \sqrt{\frac{\varepsilon \varepsilon_0}{\tau_{\text{laser}} N_{\text{abs}} e}} \eta \Sigma \mu \]  

(7)

where the maximum yield of charge carriers per absorbed photon is \( \Phi_{\text{max}} = N_{\text{max}}/N_{\text{abs}} \). This relation implies that if \( \Phi_{\text{max}} \Sigma \mu \) is constant with temperature, so is \( \eta \Sigma \mu \).

In summary, both first and second order recombination during the laser pulse cannot be the cause of a temperature independence of \( \Phi_{\text{max}} \Sigma \mu \). This indicates that it is the product \( \eta \Sigma \mu \), so the \textit{intrinsic} quantum yield of charge carrier photogeneration times the sum of the carrier mobilities, that is independent on temperature.
5. Dissociation energy of a photogenerated electron-hole pair

To estimate the dissociation energy of a photogenerated electron-hole pair we first consider the energy $E_\infty$ of a well separated electron-hole pair where the electron and hole occupy different QDs and do not interact. With respect to the unexcited QD film the energy is:

$$E_\infty = E_{1e} - E_{1h} + E_{e}^{\text{pol}} + E_{h}^{\text{pol}}$$  \hspace{1cm} (8)

Here $E_{1e}$ and $E_{1h}$ are the site energies of the electron and hole, respectively and $E_{e}^{\text{pol}}$ and $E_{h}^{\text{pol}}$ are the electron and hole self energies. When the electron and hole are brought together on a single QD the energy becomes:

$$E_{e,h} = E_{1e} - E_{1h} + E_{e}^{\text{pol}} + E_{h}^{\text{pol}} + E_{e,h}^{\text{dir}} + E_{e,h}^{\text{pol}}$$  \hspace{1cm} (9)

$E_{e,h}^{\text{dir}}$ is the direct Coulomb interaction between electron and hole and $E_{e,h}^{\text{pol}}$ is the interaction of the electron with the polarization induced by the hole, and vice versa. The dissociation energy $\Delta E_\text{diss}$ is obtained as the difference between $E_\infty$ and $E_{e,h}$ and contains the direct Coulomb interaction $E_{e,h}^{\text{dir}}$ between electron and hole, as well as the cross-polarization energy $E_{e,h}^{\text{pol}}$.

Expressions for these contributions have been derived by Delerue resulting in the following final expression for the dissociation energy:\(^3\)

$$\Delta E_\text{diss} = \frac{1.79 e^2}{4 \pi \varepsilon_0} \frac{\varepsilon_\text{in}}{R} + \frac{e^2}{4 \pi \varepsilon_0 R} \left( \frac{\varepsilon_\text{in} - \varepsilon_\text{out}}{\varepsilon_\text{in} \varepsilon_\text{out}} \right)$$  \hspace{1cm} (10)

where $\varepsilon_0$ is the vacuum permittivity and $R$ is the QD radius. Since the low frequency dielectric constant $\varepsilon_\text{in}$ of PbSe is 250\(^4\), the direct interaction term (first term in equation (10)) is very small and the dissociation energy is dominated by the second term in equation (10), which depends on the dielectric constant outside of the QDs $\varepsilon_\text{out}$. $\varepsilon_\text{out}$ is determined by the capping molecules, in this case 1,2-ethanediamine, and neighboring QDs. We consider it to be the effective dielectric constant of the film and obtain an estimate of its value by applying the Bruggeman effective medium theory:\(^5\)

$$f \left( \frac{\varepsilon_\text{in} - \langle \varepsilon \rangle}{\varepsilon_\text{in} + \kappa \langle \varepsilon \rangle} \right) = (f - 1) \left( \frac{\varepsilon_\text{m} - \langle \varepsilon \rangle}{\varepsilon_\text{m} + \kappa \langle \varepsilon \rangle} \right)$$  \hspace{1cm} (11)

Here $f$ is the fill factor of the QDs, $\langle \varepsilon \rangle$ is the effective dielectric function of the film, i.e. $\langle \varepsilon \rangle = \varepsilon_\text{out}$, and $\varepsilon_\text{m}$ is the dielectric function of the capping material. For a QD fill factor of 0.5 (corresponding to QDs with a radius of 2.0 nm, a capping layer of 0.2 nm, and a total packing density of 0.7) and using $\varepsilon_\text{in} = 250$ and $\varepsilon_\text{m} = 13.8$ for 1,2-ethanediamine\(^6\), one obtains an effective dielectric constant of 85 for the QD film. Equation (10) with an $\varepsilon_\text{out}$ value of 85 results in a dissociation energy of $\sim$11 meV.
6. Simulation of the mobility as a function of carrier density and temperature

To test whether we can explain the dependence of the activation energy on photoexcitation density without Anderson delocalization we have used a simple model that considers transport of electrons in a Gaussian distribution of energy levels. The occupation of the levels is governed by Fermi-Dirac statistics, with a Fermi level that depends on the fractional occupation \( n \) of the levels and on temperature. The assumption of thermal equilibrium can be validated by estimating the hopping rate of localized charges between adjacent QDs and using the Einstein-Smoluchovski relation. We obtain a hopping rate \( \Gamma = k_B T \mu / e \Delta^2 \) of \( 4 \cdot 10^{11} \text{ s}^{-1} \) using 4.3 nm for the distance \( \Delta \) that the carriers travel in a single hopping event, i.e. the center-to-center distance between QDs, and a mobility \( \mu \) of 3 cm\(^2\)/Vs. Since we determine the conductivity at the maximum of the transient, at a time that is determined by the temporal width of the laser pulse (~ns), all charges have undergone a large number of hopping steps. We therefore assume that the carriers have completely thermalized within the density-of-states of the QD solid.

The distribution of energy levels was modeled as a Gaussian function \( g(E) \) with a full width at half maximum (FWHM) of 40, 80, 120 or 160 meV. The occupation of the levels is governed by Fermi-Dirac statistics, leading to a fractional occupation of the density of states defined as:

\[
n = \frac{\int_{-\infty}^{\infty} f(E, E_f, T) g(E) \, dE}{\int_{-\infty}^{\infty} g(E) \, dE}
\]  

with

\[
f(E, E_f, T) = \frac{1}{\exp \left( \frac{E - E_f}{k_B T} \right) + 1}
\]

(13)

\( E \) is the level energy, \( E_f \) is the Fermi level energy and \( T \) is the temperature. For a given occupation \( n \) (that accounts for the excitation density in the experiment) and a temperature \( T \), the Fermi level \( E_f \) is numerically calculated.

Transport is assumed to take place according to the Miller-Abrahams rate:\n
\[
\Gamma(\Delta E, T) = \begin{cases} 
\Gamma_0 \exp \left( \frac{\Delta E}{k_B T} \right) & \text{for } \Delta E > 0 \\
\Gamma_0 & \text{for } \Delta E \leq 0 
\end{cases}
\]

(14)

where \( \Gamma_0 \) is an attempt rate which is assumed to be constant in the studied temperature range. \( \Delta E \) is the difference between the initial state energy \( E_1 \) and the final state energy \( E_2 \) in the hopping process.

The conductance \( G \) is obtained by integrating the charge transfer rate over all empty final states sites in the density-of-states and over all occupied initial sites for a given temperature and fractional occupation:
The average mobility $\mu$ is obtained as $G/n$ and is of arbitrary units. Fig. S6a shows the mobility vs. temperature for different values of $n$, corresponding to different excitation densities, and for a 120 meV FWHM of the distribution of states. It is clear that the trends visible in the experiment are reproduced: disorder results in thermally activated transport with an activation energy that decreases with increasing charge carrier density. Fig. S6b shows the calculated activation energy for FWHM of the Gaussian density of states of 40, 80, 120 and 200 meV. In our simulations, the activation energy does not vanish at high fractional occupation of the levels. Even for a FWHM of 40 meV, which corresponds to the width of the sharpest first excitonic transition reported in literature, the activation energy reaches a lowest value of 11 meV. The simulations strictly deal with localized states and does not allow a vanishing activation energy because there will always be a number of sites involved in charge transport with a site energy higher than the Fermi energy.

\[
G = \int \int f(E_i, E_j, T) g(E_i) (1 - f(E_i, E_j, T)) g(E_j) \Gamma(E_i, E_j, T) \, dE_i \, dE_j
\]  

(15)

**Figure S6** a) Simulated mobility as a function of temperature and fractional occupation of the levels (0.001 to 0.064). The FWHM of the density of states is 120 meV. The data points represent simulated values; the dashed lines are linear fits. b) Simulated activation energy as a function of fractional occupation of the levels (0.001 to 0.064). The FWHM of the density of states is 40 meV (cross symbols), 80 meV (circle symbols), 120 meV (triangle symbols) and 160 meV (square symbols).
7. Estimate of the temperature increase resulting from photoexcitation

At high laser fluence the amount of energy deposited into the QD film could result in an increase of the local temperature. If this increase is significant, the local temperature differs from the measured temperature of the surroundings. This would affect activation energies that are derived from the temperature dependent photoconductivity.

The temperature rise can be estimated from the number of absorbed photons per quantum dot. At an excitation density of 1 absorbed photon per QD the amount of energy stored in the QD is 1.8 eV. If it is assumed that that all energy deposited in the system is immediately converted to heat and no heat conduction to the ligands, other quantum dots or the environment occurs the increase in temperature can be evaluated from the QD diameter (3.9 nm), the density of PbSe (8.1·10³ kg/m³) and the heat capacity of PbSe (175 J/(kg·K), roughly constant over the range 90 K – 350 K). This results in a temperature increase of 6.6 K. Since the lowest temperature used in our experiments was 90 K, and since the 6.6 K is a severe upper limit to the real heating it can be discarded as insignificant.

At the highest laser fluences used in our experiments the excitation density is ~100 absorbed photons per quantum dot and, hence, the temperature increase estimated as above would be 660 K. Obviously this is a significant increase in temperature. Therefore we try to estimate the effect of heat conduction to the quartz substrate within the laser pulse duration. The power dissipated via heat conduction, \( P_q \), for a steady state situation is given by:

\[
P_q = k A \Delta T / d
\]

Here \( k \) is the thermal conductivity of the material, \( A \) is the area, \( \Delta T \) is the temperature difference over the material and \( d \) is its thickness. Since we are evaluating a transient situation rather than a steady state situation, this problem was solved numerically by dividing the system into 1 nm slabs of PbSe (35 slabs) and quartz (10⁵ slabs) and evaluating the heatflow between the slabs in timesteps of 10 fs. The results are shown in Figure S7. If a thermal conductivity of 1.4 W/(m·K) is assumed for the substrate and a thermal conductivity of 2 W/(m·K) is assumed for the QD film (corresponding to bulk PbSe), the temperature drops exponentially with a 1/e time of 0.23 ns (Figure S7a) and the photon energy is efficiently transferred to the substrate within the 3 ns duration of the laser pulse.

However, the cooling rate depends strongly on the thermal conductivity of the QD film. This thermal conductivity is unknown to us, but it has been suggested that the thermal conductivity of nanocrystal films could be much lower than that of the bulk solid. Figure S7b shows the temperature transient for thermal conductivities of the QD film of 2 (black curves), 0.2 (red curve) and 0.067 W/(m·K) (blue curve) for an excitation density of 100 absorbed photons per QD. In all cases cooling is significant during the 3 ns laser pulse, indicating that the simple temperature estimate made above is too high. However, if the thermal conductivity of the QD film is 30 times lower than that of bulk PbSe the temperature drops only by a factor of 2 in 3 ns, which means that heating due to photoexcitation will be appreciable. As long as the actual thermal conductivity of PbSe QD films is not known the temperature increase upon photoexcitation cannot be estimated more accurately.
Figure S7 Simulation of the average temperature of the QD films upon photoexcitation and the resulting cooling due to heat conduction to the quartz substrate. a) Cooling for different thermal conductivity values of the PbSe QD film at an excitation density of 100 photons per QD. In all cases the cooling is significant during the laser pulse duration of 3 ns. b) Cooling for different excitations densities at a thermal conductivity of the PbSe QD film of 2 W/(m·K).

We stress however that the trend of decreasing activation energy with increasing excitation density is very clear already at laser fluences where local heating may be neglected (roughly below 1 absorbed photon per QD). The activation energy that we determine is 4 meV at 1 photon/QD, 2 meV at 8 photons/QD, 0.8 meV at 20 photons/QD and -0.4 meV at 100 photons/QD. Our simulations included in section 5 of this supplementary information, predict that the remaining activation energy at high carrier density should be 23 meV in the case of hopping conductivity. Hence, even if the two highest fluences are disregarded it is clear that the activation energy decreases to an extent that cannot be explained in the framework of hopping conductivity.
8. Deconvolution of the Time-Resolved Microwave Conductivity transients

The photoconductance was measured with the Time-Resolved Microwave Conductivity (TRMC) technique. A microwave cavity was used to increase the sensitivity at the expense of the response time (17.4 ns), which modifies the decay kinetics at short times. This is illustrated in Fig. S8 that shows a photoconductance transient obtained for a PbSe QD film in the microwave cavity (red solid line in Figure S8) and in an open cell (blue solid line in Figure S8). The photoconductance transients were deconvoluted for the cavity response. Details on the deconvolution procedure are presented below. The deconvoluted signal (blue open circles in Fig. S8) is identical to the transient measured without cavity (blue solid line) and is limited by the 3 ns width of the laser pulse. This shows the effectiveness of our deconvolution procedure. The maximum of the deconvoluted photoconductance signal \( \Delta G_{\text{max}} \) is used to calculate \( \Phi_{\text{max}} \Sigma \mu \).

![Figure S8](image)

Figure S8: Photoconductance transients obtained at room temperature for a PbSe QD film in the microwave cavity (red solid line) and the open cell (blue solid line), and convoluted signal from the measurement in the cavity (blue open circles).

In what follows the mathematical basis of the deconvolution procedure is presented. Consider the frequency-dependent functions \( f(\omega), g(\omega), s(\omega), n(\omega) \), representing respectively the measured signal, the cavity response, the noiseless deconvoluted signal, and the noise on the data. In the frequency space they are related as:

\[
f(\omega) = g(\omega)s(\omega) + n(\omega)
\]

(17)

In time domain the above product of \( g \) and \( s \) converts to a convolution. The cavity response can be written as follows:

\[
g(\omega) = \frac{e^{-i\omega \tau_{\text{res}}}}{1-i\omega \tau_{\text{res}}}
\]

(18)

with \( \tau_{\text{las}} \) the duration of the laser pulse, and \( \tau_{\text{res}} \) the rise time of the cavity. \( \tau_{\text{res}} \) is determined from the cavity resonance curve in the dark. In time domain this response represents a broadened exponential decay.
The noiseless deconvoluted signal is written as a superposition of exponential decays, which translates to frequency domain as:

\[ s(\omega) = \sum_{k=1}^{N} \frac{\beta_k}{\gamma_k - i\omega} \]

Here, \( N \) represents the number of decay times appearing in the superposition, \( \beta_k \) the amplitudes of every single term contributing to the superposition, and \( \gamma_k \) the corresponding rate. In the deconvolution procedure the rates are fixed, and the amplitudes are optimized such as to minimize the integral:

\[ \int d\omega |g(\omega)s(\omega) + n(\omega) - f(\omega)|^2 \]

This amounts to solving the linear set of equations:

\[ \frac{\partial}{\partial \beta_m} \int d\omega |g(\omega)s(\omega) + n(\omega) - f(\omega)|^2 = 0 \]

This equation can be solved analytically by a matrix inversion:

\[ \bar{\beta} = P^{-1} \bar{v} \]

Here, the vector \( \bar{\beta} \) contains all the sought for amplitudes. The matrix \( P \) and the vector \( \bar{v} \) are defined as follows:

\[ P_{ik} \equiv \text{Re} \left[ \sum_j |g_{ij}|^2 Q_{ij} Q_{kj} \right] \]

\[ Q_{ij} \equiv [\gamma_k - ij\delta\omega]^{-1} \]

\[ v_k \equiv \text{Re} \left[ \sum_j Q_{kj} g_j f_j^* \right] \]

The subscripts \( j \) arise from the fact that our data are discretized:

\[ f_j \equiv f(j\delta\omega) \]

\[ g_j \equiv g(j\delta\omega) \]

\[ s_j \equiv s(j\delta\omega) \]

with \( \delta\omega \) the frequency interval of discretization, equal to the inverse of the total time span of the data in time domain.


6 Handbook of Chemistry and Physics, 90th edn, (Internet version, 2010).


