Theory of highly efficient multiexciton generation in type-II nanorods

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Multiexciton generation, by which more than a single electron-hole pair is generated on optical excitation, is a promising paradigm for pushing the efficiency of solar cells beyond the Shockley–Queisser limit of 31%. Utilizing this paradigm, however, requires the onset energy of multiexciton generation to be close to twice the band gap energy and the efficiency to increase rapidly above this onset. This challenge remains unattainable even using confined nanocrystals, nanorods or nanowires. Here, we show how both goals can be achieved in a nanorod heterostructure with type-II band offsets. Using pseudopotential atomistic calculation on a model type-II semiconductor heterostructure we predict the optimal conditions for controlling multiexciton generation efficiencies at twice the band gap energy. For a finite band offset, this requires a sharp interface along with a reduction of the exciton cooling and may enable a route for breaking the Shockley–Queisser limit.
In the recent decades, the photovoltaic power conversion efficiencies in solar cells have increased beyond the Shockley–Queisser (SQ) limit of 31% due to improvements in materials, device designs, and experimental techniques. Several theoretical concepts have been proposed to overcome this limit, such as multie exciton generation (MEG) or singlet fission, which can be prepared using cation exchange reactions. Our work is motivated by the results of MEG in carbon nanotube photodiodes, but we have identified a new mechanism for increasing the efficiency of MEG in type-II heterostructures.

Results

Model for a type-II nanorod heterostructure. To illustrate the core idea and to focus on the effect associated with the role of the internal field, we consider a model system of type-II NRs where both building blocks are composed of CdSe with an internal field at the interfacial region of width $\beta$ and maximal value $F = \Delta / \beta$, as depicted in the left panel of Fig. 1. While more realistic models of type-II nanostructures can be handled within the pseudopotential approach, we take the approach where the mechanism of generating multie excitons is not affected by the field strength within the noise level of the stochastic approach, which is important for establishing the dependence of the absorption onset energy on the internal field. We plot the results for a series of NRs with different internal fields. As can be seen clearly, the absorption onset is independent of the internal field strength within the noise level of the stochastic approach, consistent with the small overlap of the hole and electron wave functions when they are localized on opposite sides of the NR. Moreover, the entire line-shape is very similar for different values of $\Delta$. Here, we demonstrate that the absorption onset energy, most importantly the onset energy $E_{on}$, does not change with the internal field.

MEG efficiencies in a type-II nanorod heterostructure. We now proceed to evaluate the MEG efficiencies of this system. MEG is a complicated many-body problem involving singly and doubly excited states and their decay via electron–phonon couplings. Progress can only be made with well-defined, controlled approximations. We have recently shown that the direct absorption approach or indirect absorption approach, the coherent reduced density matrix formalism, and the impact excitation model all emerge as different limits of a Green’s function formalism. The impact excitation model proved to be accurate in comparison with a more elaborate Green’s function approach while providing a simple physical picture in which MEG efficiencies become notable if their rates are larger than the competing exciton cooling rates. Furthermore, the MEG process can be described to lowest order in the
Coulomb coupling as a decay of an electron/hole to a negative/positive trion state (composed of two electrons and one hole or vice versa), while the other carrier (hole/electron) is a spectator. For these reasons we adopt the impact excitation approach and implement a stochastic method developed in refs 31, 44 to overcome the computational complexity of calculating MEG rates in systems with thousands of electrons.

For completeness, we briefly review the approach and the key elements in describing the MEG efficiency \( n_{\text{ex}}(\omega) \), the number of excitons per absorbed photon. This can be written as an average over sampled electron–hole pair excitations, \( S \):

\[
n_{\text{ex}}(\omega) = \frac{1}{N_{S}} \sum_{S} P_S(\omega) \frac{2 \Gamma_S + \gamma}{\Gamma_S + \gamma}
\]

where \( N_{S} \) is the number of sampled excitons (typically \( N_{S} = 200 \) is sufficient to converge the results), \( E_S = \hbar \omega \) is the photon and exciton energy, \( \gamma \) is the exciton cooling rate taken to be energy independent, \( \Gamma_S \) the MEG rate for exciton \( S \), and \( P_S(\omega) = \rho(\varepsilon_s) \rho(\varepsilon_h) P_\omega(\omega) \) (where \( \rho(\varepsilon) \) is the density of states at energy \( \varepsilon \)),

\[
P_\omega(\omega) = \frac{1}{\omega} \sum_{\varepsilon} |\mu_{\omega\varepsilon}|^2 \delta(E_S - \hbar \omega)
\]

is the probability of generating exciton \( S \) given that a photon of energy \( \hbar \omega \) was absorbed. In the above, \( \mu_{\omega\varepsilon} \) is the transition dipole from the ground state \( |0\rangle \) to an excitonic state \( |S\rangle \). Finally, the MEG rates, \( \Gamma_S \), are given in terms of a sum of negative \( (\Gamma^-_S) \) and positive \( (\Gamma^+_S) \) trion formation rates \( \Gamma_S = \Gamma^-_S + \Gamma^+_S \), where

\[
\Gamma^-_S = \frac{2\pi}{\hbar} \sqrt{W_{\text{ch}}^2 + \rho^- S(\varepsilon_e)},
\]

\[
\Gamma^+_S = \frac{2\pi}{\hbar} \sqrt{W_{\text{ch}}^2 + \rho^+ S(\varepsilon_h)}
\]

and \( \sqrt{W_{\text{ch}}^2} \) and \( \rho^- S(\varepsilon_e) \) are the average screened Coulomb coupling and the density of trion states, respectively. All the required quantities can be obtained within the pseudopotential approach using the stochastic MEG method.

In Fig. 2 we plot the calculated MEG efficiencies for a series of NRS with varying internal fields (left panels) and varying exciton cooling rates (right panels) as a function of the photon energy \( E = \hbar \omega \). Consistent with above discussion of the onset of absorption, we scale the photon energy of all NRS with the band gap of the unbiased system, \( E_g = 2.04 \text{ eV} \). The left panel of Fig. 2 illustrates an important result, where the onset energy for MEG, \( E_{\text{on}} \), decreases markedly with the bias potential. Furthermore, comparing the results of the upper and lower left panels of the figure it is clear that a much larger effect is obtained when the length scale for the bias drop is small, namely for a large field. This latter result is consistent with theoretical predictions of the suppression of Auger processes in core-shell nanocrystals, where a sharp interface between the core and shell leads to faster Auger recombination.

Above a certain threshold value of \( \Delta \), the onset energy of MEG can be smaller than \( 2E_g \). This results explains an exploration since the minimal double-exciton energy is twice the energy of the gap, \( E_g \). To explain this seemingly unrealistic result, we sketch two possible relaxation mechanisms for generating multie excitons in the upper panel of Fig. 3. Consider an electron at high energy delocalized along the entire NR. The electron can either generate a negative trion where all carriers are localized in one building block, or can generate a negative, charge separated, trion. On the basis of energy conservation considerations, in the former the theoretical onset of MEG is \( E_g = \Delta \) while in the latter it is \( E_g = 2 \Delta \). Thus, due to the potential drop the onset can be pushed below \( 2E_g \). We note that for the charge separated negative trion, the hole orbital must overlap one of the final electron orbitals. The lower panel of Fig. 3 illustrates that this can indeed happen. However, this overlap is rather small and the central contribution comes from the localized trion state. We conclude that the dominant mechanism will push the theoretical onset energy to \( 2E_g - \Delta \).

### Analysis of the multie exciton generation efficiencies

While a finite value of \( \Delta \) is required to separate the charge carriers in type-II solar cell junctions, the value of \( \Delta \) used to increase the MEG efficiency as depicted in the left panels of Fig. 2, will lead to a significant decrease in the photovoltage and as a result, to an overall lower solar cell performance. As shown in the right panels of Fig. 2, this issue is mitigated when the exciton cooling lifetime is increased above 10 ps (which, in fact, can be induced by an pronounced electron–hole charge separation), leading to a MEG onset energy below \( 2E_g \) even at moderate values of \( \Delta \).

It is clear, however, that only by combining a non-negligible internal field and a mechanism to slow down the cooling of excitons by phonon emission, the MEG efficiency can be controlled at the desired onset, while either one of these mechanisms separately will not be sufficient.
Figure 2 | MEG efficiencies for a type-II nanorod heterostructure. (a,b): Plots of the biexciton generation efficiency as a function of energy for several different value of $A$. The cooling rate is $\gamma = 1$ ps$^{-1}$ and the range parameter is $\beta = 2.5$ nm for (a) and $\beta = 1$ nm for (b). Note that the results for the two lower values of $A$ for $\beta = 2.5$ nm are similar to those of $A = 0.45E_g$, and thus are not shown. Insets show the valance band maximum and conduction band minimum energies along the rod axes. (c,d): Plots of the biexciton generation efficiency as a function of energy for different values of $\gamma$ (the exciton cooling rate) for $A = 0E_g$ (c) and $A = 0.45E_g$ (d).

The increase of MEG rate near $2E_g$ is further analysed in Fig. 4, where we plot the DOTS (upper panel) and the average Coulomb coupling for electrons (lower panel). The density of negative and positive trion states ($\rho^+_{-e}$ and $\rho^+_{+h}$, respectively) is plotted along the positive and negative energies, respectively. Each is measured from the bottom/top of the conduction/valence bands of the unbiased CdSe NR. The DOTS is obtained by a triple convolution of the DOS not shown here. For the negative DOTS, the triple convolution involves the DOS of two electrons (that is, the DOS above the Fermi energy) and one hole (that is, the DOS below the Fermi energy) while for the positive DOTS it involves the triple convolution of the DOS of two holes and one electron. Common to both DOTS is the increase in $\rho^+_{+e}$ at $\varepsilon = \pm E_g$ above/below the conduction/valence band minimum/maximum. Note that we use a semi-logarithmic scale and thus, the magnitude of the effect is rather dramatic with increasing bias. The positive DOTS is typically higher than the negative DOTS at the energies measured from the corresponding band edge, a result that can be explained by the larger DOS of holes$^{44}$. Furthermore, the negative DOTS shows a stronger dependence on the internal bias potential.

The increase in the DOTS at energies $\pm E_g$ above and below the corresponding band extremes is a necessary but not sufficient condition for pushing the onset of MEG to $2E_g$. In addition, the coupling of the excited electron–hole pair need not vanish. While the average Coulomb coupling for electrons shown in the lower panel of Fig. 4 is nearly independent of energy at high energies, consistent with the picture emerging for NCs (ref. 31) and NRs (ref. 38), in the important range of $\varepsilon \approx E_g$ there is a notable small increase in $\sqrt{|W^2_g|}$ as the internal field is increased due to a change in the character of the trion states to which the electron (hole) is coupled. The increase in the DOTS and in small increase in $\sqrt{|W^2_g|}$ leads to a significant soaring of the trion formation rate above the exciton cooling rate, $\gamma$. This interplay of DOSs and Coulomb coupling and the energy dependence is reflected in an increase of MEG efficiencies and a decrease of $E_{\text{cond}}$ as discussed above.

In summary, using MEG in nanostructures for breaking the SQ limit requires a significant increase in the MEG efficiencies at $2E_g$. So far, this has been elusive and neither spherical NCs nor core-shell NCs nor NRs push the onset of MEG to $2E_g$. Here, we provide the theoretical foundation for the design of materials with large MEG efficiencies near $2E_g$. Our predictions are based on an atomistic model for MEG within a fully quantum mechanical description, which has been shown to be accurate in postdicting and predicting MEG in NCs and NRs. The two key elements for pushing down the MEG onset energy are: (a) Using the internal field ($A/\beta$) in type-II heterostructures with a rather sharp interface between the two building blocks and (b) slowing down the exciton cooling rate by reducing the electron–phonon
DOTS are plotted on negative energies and the negative (electron) DOSs are plotted on positive energies. Moderate value of the band offset, one requires the design of materials with gaps close to 0.7 eV.

Methods

Computational method. All calculations were preformed within the pseudopotential model for CdSe (ref. 47) implemented in a real-space grid of size $96 \times 96 \times 384$ and spacing of 0.8 a.u. sufficient to converge the results. The NR included 3,600 Cd and 3,600 Se atoms and ligand potentials were used to passivate the dangling bonds. The description of the electronic properties of this system is beyond the current capabilities of deterministic approaches. Therefore, we resort to our recently developed stochastic formalism. For the MEG efficiency given by equation (1) we have carried the following steps:

First, the DOSs, $\rho(\epsilon)$, were obtained using a stochastic trace formula with an interpolation polynomial of length $N_S = 16,384$ averaged over 50 stochastic iterations. The positive and negative trion DOSs ($\rho_T(\epsilon)$, $\rho^*(\epsilon)$) were then generated by a triple convolution of the single-particle DOSs. More details are given in ref. 31. Next, negative and positive trion formation rates in equation (3) were generated using a stochastic procedure. This involves filtering electron and hole states at a target energy and filtering a resonant negative and positive trion state, respectively, using an interpolation polynomial of length $N_S = 16,384$. For each interpolation polynomial filter we have generated 16 electron states and 16 hole states and for each particle a corresponding resonant trion state. The rates were averaged over 10,000 stochastic realizations. In addition, for each electron or hole obtained in the previous step, we have filtered several (10) hole or electron states, respectively, and for each electron–hole pair we calculated the transition dipole $\mu_{ij}$ at energy $E_f$ and obtained $W_f(\epsilon)$ given by equation (2). Since we only sample electron–hole pairs, instead of calculating them all, we have multiplied the result by the density of electrons and holes $\rho(\epsilon)$ at the reference energy of the electron ($\epsilon_e$) and hole ($\epsilon_h$). For more information see ref. 44. Finally, we have used $F_T$ and $F^*$ to generate the MEG rate for each excitation: $F_T = F_T^o + F_T^h$ and then obtained $\sigma_T(\epsilon)$ by performing the average in equation (1) for $N_T = 50,000$.

The absorption cross section, $\sigma(\epsilon) \propto \text{or}(\epsilon)$ is given in terms of the golden rule absorption rate, $r(\epsilon) = \frac{\pi}{\hbar} \sum_{ij} \int \text{d}t \epsilon^2 S(\mu(0); 0(1))|\psi_0(0)|^2 S(\mu(1); 0(1))$, where $\mu$ is the dipole operator, $S$ is the amplitude of the electromagnetic field, $|0(0)|$ is the ground state and $|5|$ is an electron–hole pair state. Instead of summing overall electron–hole pairs, an impractical task for the studied NR size, we used the following stochastic formula: $\sigma(\epsilon) = \frac{\pi}{\hbar} \sum_{ij} \int \text{d}t \epsilon^2 S(\mu(0); 0(1))|\psi_0(0)|^2 S(\mu(1); 0(1))$, where $\psi$ is a projected random orbital on the occupied space and $\psi$ is a project random orbital on the unoccupied space (see more details about random stochastic orbitals in ref. 51). We used $N_T = 10,000$ to average the rate of absorption and $N_T = 10^9$ propagation steps with a time step of 0.025 a.u. to propagate the electron–hole stochastic orbitals.

Data availability. The data that support the findings of this study are available from the corresponding authors on request.

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Authors contributions
H.E. performed the calculations and analysed the data, R.B., D.N. and E.R. developed the theoretical framework and analysed the data, all authors co-wrote the paper.

Additional information
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