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***Abstract*—Among many material candidates for next-generation solar cells, quantum dots offer unique opportunities. Aiming to maximally harness their nanoscale bandgap engineering, in this work we outline a multiscale, multiphysics modeling approach for the device level simulation of quantum dot solar cells. Examples of experimental validation are discussed, emphasizing the potential of light trapping techniques towards the implementation of quantum dot based intermediate band solar cells.**

I. Introduction

One of the hottest concepts in photovoltaics is the intermediate band solar cell (IBSC). The IBSC can be regarded as a tandem cell at the nanoscale where, as shown in Fig. 1(a), the presence of an intermediate energy level within the forbidden bandgap of a host semiconductor allows to split the sun harvesting over different energy transitions, enabling efficiency well above the Shockley-Queisser (SQ) limit of a single gap solar cell [1].

Thanks to their tunable electronic and optical properties, quantum dots (QD) are an ideal platform for IBSC, where the IB is created through the intraband energy levels introduced by the 3D carrier confinement. The most studied systems so far pertain the III-V semiconductor family, in particular InAs QDs self-assembled in a GaAs matrix [2]. Fig. 1(b) schematically shows the IB operation for such QD system. Besides the band-to-band absorption of the host semiconductor, the QD states enable the absorption of below gap photons, increasing the short circuit current density (J_{sc}) [3]. However, to overcome the SQ limit of a single gap cell, this J_{sc} increase must be larger than the reduction of the open circuit voltage (V_{oc}) caused by the narrower effective bandgap of the QD region. This reflects into the requirement for the bulk carriers IMREFs to be separated from the QD ones, i.e., a non-equilibrium condition must exist between extended and confined carrier states, sustained by the energy provided by the incoming sunlight. Key to this process is the two-step photoexcitation of carriers in the extended bands through a two-photon sequential absorption process, or hot phonon assisted carrier escape promoted by the absorption of high energy photons [4]. As opposite, see Fig. 1(c), relaxation of bulk carriers into the QD states and conversely thermal (or field-assisted) escape from the QDs to the extended band states bring the two ensembles towards equilibrium, making the cell to work as a single junction cell, with V_{oc} limited by the QD effective gap. QDSCs operating in such thermally-limited regime have potential applications in space and low cost concentration systems [5], [6].

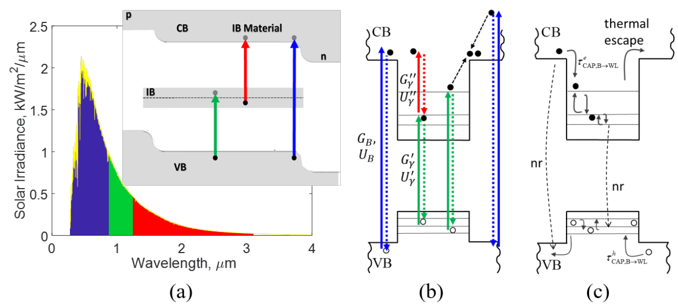

Fig. 1. Intermediate band solar cell concept (a) and its implementation in a QD stack with indication of (b) photon assisted inter- and intra-band processes sustaining IB operation, (c) thermal assisted capture/escape hindering the IB operation and non radiative recombination.

State of art devices are in fact mastered by thermally assisted processes, the low QD optical cross-section being at the root of this problem. This is why the demonstration of a practical QDSC operating in the IB regime has yet to come. Overcoming this scenario would require increasing the QD volume occupation by a $100\times$ factor, which is technologically unaffordable, especially in view of minimizing non-radiative recombination [7]. A promising alternative path to increase the optical path length at the QD wavelengths without compromising the crystal quality, is resorting to light trapping approaches [8], e.g. by implementing diffraction gratings within a thin-film architecture [6], [9].

From this brief overview it is clear that physics-based device modeling and simulation of QDSCs is a formidable task since it requires to deal with a truly multiscale and multiphysics problem, encompassing both material- and device-level aspects. In this work, we summarize our recent work on the device level modeling of QD solar cells at transport and photonic level, with an overview of the modeling approaches and their experimental validation.

II. Modeling Approaches and Results

From the transport point of view, QDSCs can be accurately described by semiclassical transport-based models corrected

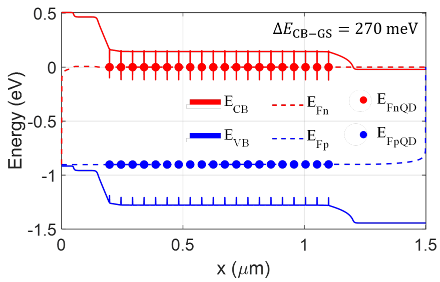

Fig. 2. Energy ban diagram at V_{oc} for an InAs/GaAs QD solar cell with 18 e/dot direct doping [11], [10] for non-radiative recombination suppression.

with a proper description of the QD interband and intraband carrier processes depicted in Fig. 1, and accounting for electrostatic effects due to charge localization in the QDs. The modified electron continuity equation in steady state reads as

$$\frac{1}{q}\frac{\partial J_n}{\partial x} = U_{\mathrm{B}} - G_{\mathrm{B}} + \sum_{\gamma} U''_{\gamma} - \sum_{\gamma} G''_{\gamma} + U_{n,\mathrm{CAP}}, \quad (1)$$

where U_{B} and U''_{γ} are the net inter- and intra-band recombination rates (including both radiative and non-radiative processes) of bulk and sub-band states (i.e. $\gamma =$ WL, ES, GS for a three-level QD model), respectively, G_{B} and G''_{γ} the inter- and intra-band photogeneration rates, and $U_{n,\mathrm{CAP}}$ the net capture rate from the barrier to the WL state. Capture and cascaded relaxation processes are described by a set of space-dependent equations imposing, for each energy level, a detailed balance among all the charge transfer mechanisms:

$$U_{n,\mathrm{CAP}}^{\gamma+1\to\gamma} - U_{n,\mathrm{CAP}}^{\gamma\to\gamma-1} - U'_{\gamma} + G'_{\gamma} + U''_{\gamma} - G''_{\gamma} = 0. \quad (2)$$

The net capture rate results as [10]

$$U_{n,\mathrm{CAP}}^{\gamma\to\gamma-1} = \frac{1}{\tau_{\mathrm{cap}}^{\gamma-1}} n_{\gamma} \left(1 - \frac{n_{\gamma-1}}{N_{\gamma-1}}\right)\left(1 - \mathrm{e}^{\dfrac{E_{Fn}^{\gamma-1} - E_{Fn}^{\gamma}}{k_B T}}\right),$$

n_k and N_k being the free electron density and effective density of states of the k subband, with the characteristic capture time $\tau_{\mathrm{cap}}^{\gamma-1}$ describing the interaction between the γ and $\gamma - 1$ subbands. Eq. 2 evidences the competition between thermal and photon-assisted processes.

Fig. 2 shows an example of energy band diagram at open circuit condition for an InAs/GaAs QDSC operating in the thermally-limited regime, characterized by the pinning of the IMREFs in the highly doped contact layers to the QD IMREFs and, consequently, by a significant reduction of the attainable V_{oc}. Photogeneration is calculated according to the optical cross-section and states occupation. From the photonic point of view, wave-optics approaches are needed for thin-film architectures: 1D for planar devices, 2D or 3D models for patterned surfaces. Frequency-domain approaches such as rigorous coupled wave analysis (RCWA) are particularly suitable for periodic diffraction gratings. When electro-optical self-consistency is required to take into account of carrier density-dependent optical properties and include photon recycling effects, semi-analytical multimodal field expansions can be used to reduce the computational burden [12]. Effective photon management can significantly relax the requirements in terms of QD stack density and concentration factor required for IB operating regime. As an example, Fig. 3 compares the thermal- and photon-assisted net escape rates for type-II GaSb/GaAs QDSCs [13], [14] in a conventional wafer based configuration and in a thin-film light-trapping enhanced cell. In the latter, optical escape overcomes the thermal one at about one order of magnitude lower concentration, highlighting the potential of photon management to implement practical QD-IBSCs.

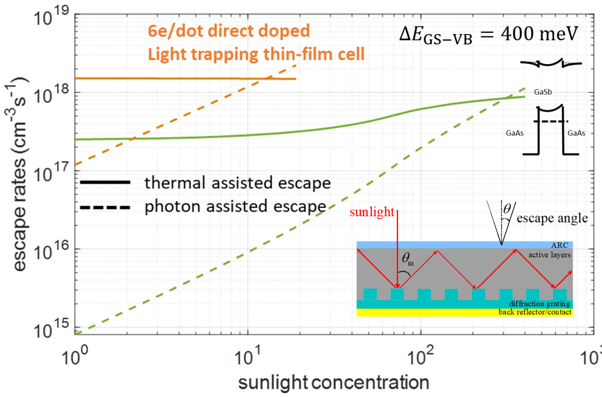

Fig. 3. Competition between thermal and photon assisted escape rates as a function of the concentration factor in a GaSb/GaAs QDSC: (a) on wafer and (b) thin-film with a light trapping scheme enabling 25 increased absorptivity in the weak absorption limit. The insets show the GaSb/GaAs energy bands and a sketch of a thin-film cell with rear diffraction grating for light trapping.

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