Interlinked impacts of tunneling and optical couplings in a QD-based photovoltaic nanocell

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INTRODUCTION

In next generation solar cells, quantum dots (QD) may be used to increase efficiency compared to conventional solar cells [1] thanks to quantum confinement. The simulation of such quantum devices needs to rely on advanced theories such as non-equilibrium Green's function [2]. In this work, we use this kind of simulations to examine the carrier photogeneration in a QD connected to two quantum wires (QW) at each side schematically represented in Fig. 1(a).

NANOCELL SIMULATION

We developed a mesoscopic two-orbital tight-binding model in which QD states replace the atomic orbitals. Band diagram is given Fig. 1(b). With this nanocell diagram, the dark current is very small compared to the photocurrent, it is hence ignored here. The transport properties were calculated within the NEGF formalism in which self-energy functions account for interactions. Details on the simulation can be found in former studies [3]. We include the electron-photon interaction in the self-consistent Born approximation. The interaction parameter is here the optical coupling M. Each QD-QW contact is described by a contact self-energy. The contact parameter is the tunneling coupling h, equal for the two contacts and the two bands. In a previous work, we showed a counterintuitive response of the cell: the I-V curve exhibits a negative differential conductance [4].

We now propose to deeper examine how the nanocell design can impact its response under a monochromatic radiation. We thus examine the carrier photogeneration depending on the relative strengths of the two couplings h and M. In this work, the contact self-energies were simplified compared to our previous studies using the wide band limit (WBL), and they are represented Fig. 2.

NANOCELL RESPONSE

The nanocell exhibits several regimes of carrier photogeneration Fig. 3: the short-circuit current is either increased by an increase of a coupling (the other one remaining fixed), either decreased. In Fig. 3(a) above the dashed cyan line D_h, increasing the tunneling coupling h surprisingly decreases the current, for a given optical coupling M. Close to point A, there is the strong tunneling regime. While below D_h, increasing h increases the current, as intuitively expected. In Fig. 3(b), the black dashed line called D_M also evidences two zones. At the left hand side of D_M, increasing M increases the current at given h. However, at the right hand side of D_M, still increasing M surprisingly damages the current.

The increase of the short-circuit current in the Fig. 3a above D_h is related to the negative differential conductance explained in Ref. [4]. Indeed, above D_h, increasing h diminishes and enlarges the spectral response of the dot: the photogeneration reduces. At the right hand side of D_M, increasing M enlarges the dot spectral response which is finally cut by the QW band edges following the same mechanism of NDR in resonant tunneling diode.

For instance, current mappings shown Fig. 4 reveal that the nanocell still exhibits a resonance as a function of the photon energies, which depends on the strength of h: strong in Fig. 4(a) and weak in Fig. 4(b).

CONCLUSION

Using NEGF, we demonstrated strong and interlinked impacts of tunneling and optical couplings on carriers photogenerated under monochromatic light in a nanocell made of a QD connected to two QWs. We believe this work also provides matter for new proposals in nanophotovoltaics.

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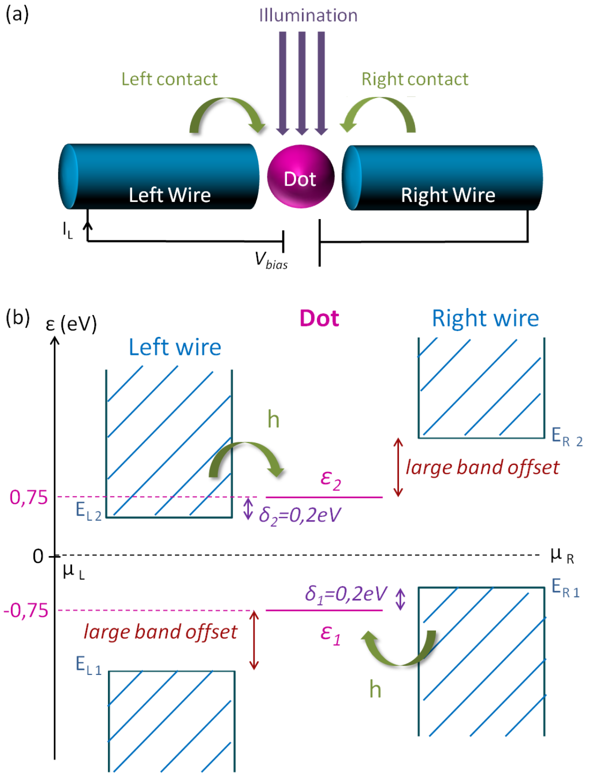

Fig. 1. a) Scheme of the photovoltaic nanocell. (b) Band diagram of the unbiased junction: two discrete energy levels are available in the dot at energies ϵ_1 and ϵ_2. Electronic states in the wires are given by two wide bands (VB and CB). Electron/hole selectivity is supported by large band offsets at the left VB and right CB contacts.

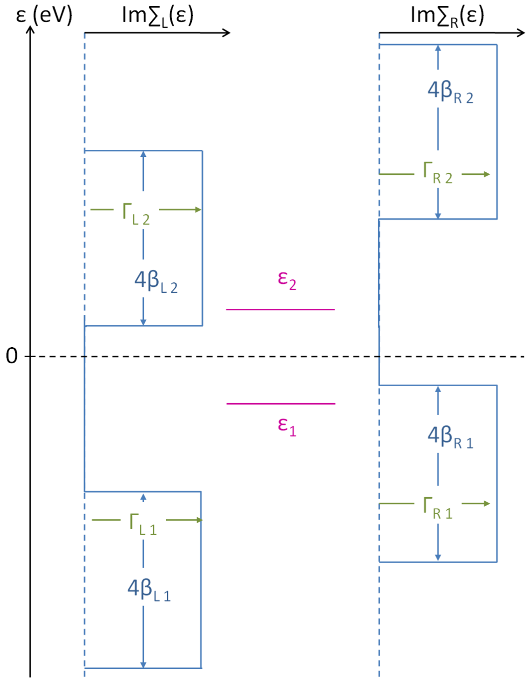

Fig. 2. Self-energies Σ_L and Σ_R at the left and right QD-QW contacts in the WBL approximation.

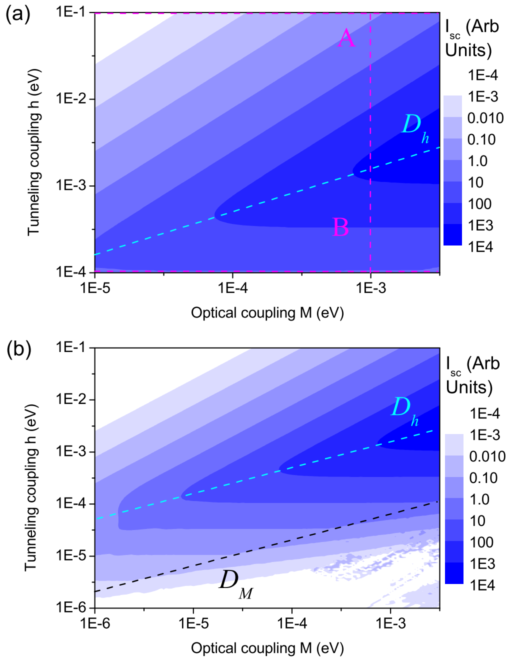

Fig. 3. (a) and (b) Left short-circuit current as a function of the tunneling coupling h and the optical coupling M. Photon number values $n_\gamma = 2.077\ 10^{-11}$.(a) is a zoom of (b). The point A has for coordinates ($M = 10^{-3}\ eV$,$h = 10^{-1}\ eV$) while the B has for coordinates ($M = 10^{-3}\ eV$,$h = 10^{-4}\ eV$). The two dashed lines, D_h in cyan and D_M in black, are parallel. They are guides for the eye and highlights the several zones of each figure.

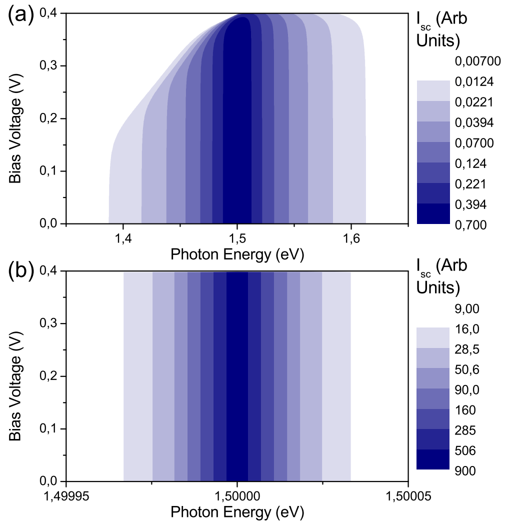

Fig. 4. (a) Left Current production in zone A as a function of the bias voltage V_{bias} (V) and the photon energy $\hbar\omega$ (eV). Here: $h = 0.1$ eV and $M = 10^{-3}$ eV. (b) Current production in zone B. The current is plotted as a function of the bias voltage V_{bias} (V) and the photon energy $\hbar\omega$ (eV). Here: $h = 10^{-4}$ eV and $M = 10^{-3}$ eV. For both figures, photon number values $n_\gamma = 2.077\ 10^{-11}$.