# Theoretical model of quantum dot array based intermediate band solar cell

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## MODEL

We present a theoretical model for design and analysis of semiconductor quantum dot (QD) array based intermediate-band solar cell (IBSC) [1]. The plane-wave method with periodic boundary conditions [2] is used in expansion of the **k·p** Hamiltonian for calculation of the electronic and optical structures of InAs/GaAs QD array. Taking into account realistic QD shape, QD periodicity in the array, as well as effects such as band mixing between states in the conduction and valence band, strain and piezoelectric field, the model reveals the origin of the intermediate-band formation inside forbidden energy gap of the barrier material. Having established the interrelation between QD periodicity and the electronic structure across the QD array's Brillouin zone, conditions are identified for the appearance of pure zero density-of-states regions, that separate intermediate band from the rest of the conduction band.

## RESULTS

For typical QD array QDs, Fig. 1, we have estimated energy gaps between valence band (VB) and intermediate band (IB) of 1.2 eV and between IB and conduction band (CB) of 0.124 eV. Our predictions suggest that the most promising design for an IB material that will exhibit its own quasi-Fermi level is to employ small InAs/GaAs QDs (~6-10 nm QD lateral size) [3]. With appropriate design of the QD array structural parameters: (1) it is possible to achieve the regions of pure zero DOS between IB and the rest of the CB states, that is desirable for "photon sorting" and increased efficiency of device, and (2) it is possible to achieve the strong optically allowed excitation between IB and CB, Fig. 2 [4]. Analysis of various radiative and nonradiative times indicates that: (i) the ratio between CB to IB and IB to VB radiative times is ~50, (ii) although phonon related relaxation time between CB and IB (56 ns) amounts to a half of the radiative relaxation time between CB and IB (109 ns), it is still one order of magnitude larger than the IB to VB radiative time (2.1 ns), (ii) nonradiative phonon absorption process that promotes electrons from IB to CB is very slow (650 ns) and probably would not significantly affect the transport properties of the IBSC, (iv) nonradiative Auger bi-exciton relaxation time (8.4 ns) is longer then radiative IB to VB relaxation time, indicating that this process will still be predominately radiative, (v) most detrimental effect on transport properties can originate from non- radiative Auger electron cooling process (2 ps), that is three orders of magnitude faster than any other relaxation process in the IBSC [4]. Special attention needs to be paid in the design of the IBSC structures in order to suppress the effects of electron cooling and to provide an increased efficiency of the IBSCs. Under radiative-limit approximation, that might be questionable here, we have estimated efficiency of such IBSC to be no larger than 34%, Fig 3.

The typical decay rate associated to Auger electron cooling process in InAs/GaAs QDs has been calculated to be in the range of 1-10 ps (in very good agreement with other theoretical and experimental results). Such fast decay could jeopardize the quasi-Fermi level separation between CB and IB, and in turn the voltage preservation in the IBSC. If the excitonic gap between IB and VB has to be preserved to maintain the good IBSC open circuit voltage, an alternative way to mediate the electron cooling rate is to reduce the overlap between the wave functions in the IB and VB. We further compare the Auger electron cooling times in realistic InAs/GaAs QDs with those in an idealised structure in which the valence band offset (VBO) between InAs QD and GaAs barrier is set to zero, i.e., in VB confinement-less structure. Although

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idealised, such a structure shows increase in the Auger electron cooling rate in the range of ~1 ns to ~8 ns. In this way we have shown theoretically that, with appropriate band structure engineering, it is possible to place the intraband Auger electron cooling decay timescale in the ns range, the same range of other radiative processes.

The same effect, of increasing the Auger electron cooling time, can be archived using week type-II heterostructures. In such a structure the electron and hole wave functions are spatially confined in different regions. Such an realistic and optimized design requires a Sb containing GaAsSb alloy for in the barrier region in order to induce the type-II alignment (Sb > 18%) and spatial electron/hole separation. Moreover in InAs/GaAs QD on GaAsSb buffer the rediative time between IB and VB is increased to micro second range, the same range as the intersubband radiative time between CB and IB. Also the detrimental Auger electron cooling is increased to ~0.1 ns, Fig. 4. Our theoretical predictions show excellent agreement with recent experimental measurements [6,7] on the same structures. Simultaneous increase of both times, comparing to InAs/GaAs QD, can help to provide for much better electron dynamics between CB and IB in IBSC, and preservation of the CB to IB quasi-Fermi level separation under realistic operation conditions.

## ACKNOWLEDGMENT

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## REFERENCES

[1] A. Luque, A. Marti, and C. Stanley *Nature Photonics* **6**, 146 (2012)
[2] S. Tomić, in *Next Generation of Photovoltaics*(Springer, Heidelberg 2012)
[3] S. Tomić, T.S. Jones, N.M. Harrison, Appl. Phys. Lett. **93**, 263105 (2008)
[4] S. Tomić, Phys. Rev. B **82**, 195321 (2010)
[5] S. Tomić, A. Luque, A. Marti, L. Antolin, Appl. Phys. Lett. **99**, 053504 (2011)
[6] S. Tomić, T. Sogabe, Y. Okada, Prog. Photovoltaics, in press (2014)
[7] K. Nishikawa et al, Appl. Phys. Lett. **100,** 113105 (2012)

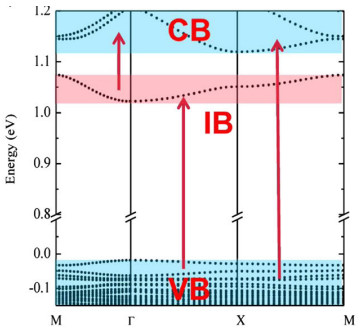


Fig. 1. Electronic structure of the laterally coupled 2D QD array throughout the 1st BZ: (a) array made of QDs with b=10nm and dx =dy =1nm

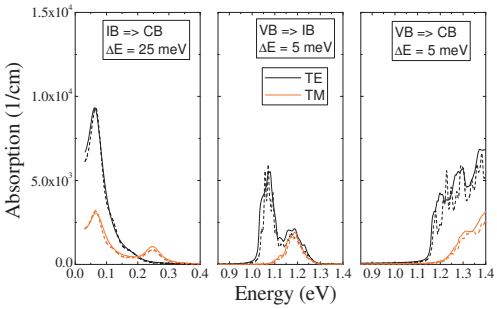


Fig. 2. Absorption coefficients of the laterally coupled 2D QD array made of QDs with b=10nm and dx =dy =1.

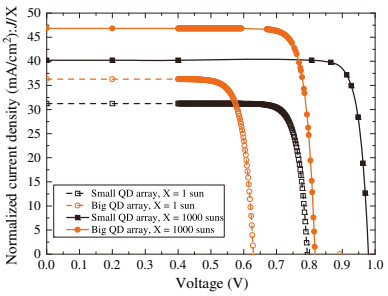


Fig. 3. The I-V curves for two different QD arrays considered in the main text and different light concentrations.

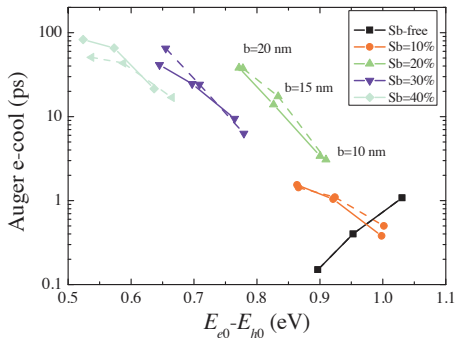


Fig. 4. Auger electron cooling time of an electron in e1 state relaxing to e0 as a function of transition energy between e0 and h0 ground states and Sb concentration in buffer region.