Modeling the influence of the dot size distribution on the line shape of the quantum dot based solar cell.

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Abstract: Photovoltaic technologies have been improving over the last years mainly due to advances in the area of nanotechnologies. Multi-junctions solar cells have reached the largest efficiencies of light conversion (around 40 %) under laboratory conditions due to the fact that junction materials might be tuned to work for wider solar bands than single junction cells. At the same time, quantum dot based composites solar cells have emerged as promising candidates to increase the conversion efficiency and durability of operation. In this communication, the effect of the dot size distribution on the photoemission line shape of a quantum dot based composite solar cell is addressed. Three different types of size distribution (homogeneous, Gaussian, and power law) are considered and the photoemission spectrum is calculated as the convolution of the emission from a single quantum dot and the distribution function of their sizes within the composite. Despite of the qualitative agreement with experimental findings there are quantitative differences due to the omission of near field effects when dots are heavily packed and resonance phenomena due to Plasmonic resonances.

Keywords: *nanotechnology, quantum dots, photovoltaic cells, optical response, dot size distribution function.*

Introduction

The increasing energy demands of modern societies and the negative effects of fossil fuels on the environment despite of their concentrated output define two of the main challenges to be addressed by materials science and environmental engineering in order to secure a long term sustainable development. The production of electricity faces also another problem, the increasing urbanization, which creates an imbalance between highly, and populated urban areas and sparse populated rural ones demands from electric grids a smart distribution and control of the loads. Moreover, the cabling in rural areas makes the process of maintenance and distribution somehow inefficient. A better and optimal use of the solar energy might be the possible solution to such challenges. Different approaches have been adopted to enhance the conversion efficiency of the photovoltaic cells (PVC). Multi-junction cells take advantage of different wavelengths of the solar spectrum, however, most of them use toxic chemicals as components. A potential improvement is coming from nano-structured materials, for instance, quantum dots. Quantum dot based solar cells also take advantage of different sections of the solar spectrum. It is conditioned by the sensitivity of quantum transitions and photo-generation on the radii of quantum dots. Therefore, controlling the distribution of quantum dot sizes it is possible to access a wide range of the solar spectrum and to improve the photo-conversion process.

This communication is aimed at exploring the impact of the distribution of quantum dot sizes on the optical response of quantum dot based solar cells. Three types of dot sizes distributions are considered: A homogeneous, a Gaussian with a characteristic size and spread, and a power law with no characteristic size. It is hypothesized that the dot size distribution is controlling the efficiency of the photocells along with the intrinsic physical quantities.

Model and Results

A composite matrix containing quantum dots of spherical shape is considered. The distribution of radii of these quantum dots (QDs) is assumed to be one of the following options: An homogeneous distribution, with QDs with radii ranging from a minimum to a maximum value with equal probabilities, a Gaussian distribution of radii with a characteristic value and some standard deviation due to fluctuations during the growth process, and finally a power law distribution with no characteristic size and decreasing for large values.

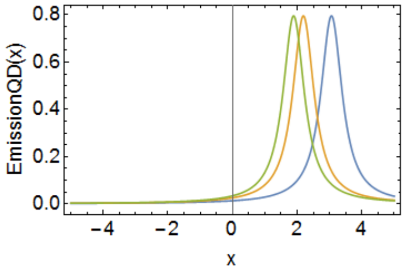

Fig 1: Emission spectrum of a QD for three different radii. The variable x, is the energy difference between levels.

Solving the Schrodinger equation for a single QD in spherical coordinates with the help of Wolfram Mathematica, the energy of the transition can be computed as a function of the QD radius. Assuming a Lorentzian shape for the emission spectrum and substituting the obtained excitation energies, the curves are presented in Fig 1 (blue line corresponds to the smallest radius, while the green one the largest radius). The emission from the whole composite matrix was represented as the convolution of the Lorentzian emission curve for a single QD times the probability distribution function (PDF) of the QD radii. Results are presented in Fig. 2.

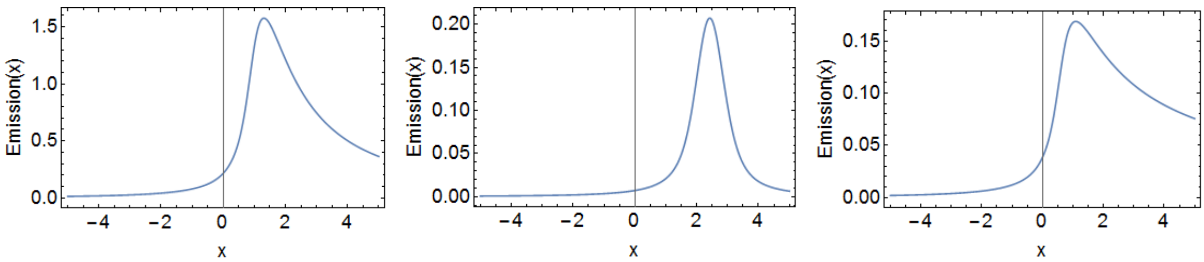

Fig 2: Emission spectrum of the QD obtained for three different distributions of radii: (Left) homogeneous, (Middle) Gaussian, and (Right) Power Law

It is worth to notice some limitations of this study: QDs geometries may differ from the spherical one. They may potentially be ellipsoids and needles; the emission spectrum from a collection of QDs should consider the effects of self-interference from different QDs emitting simultaneously as well as the tunneling between QDs is neglected.

Conclusions

There is valuable information about the distribution of radii in the QDs-based PVC within the emission line-shape. The line-shape control might constitute a method for quality control when QDs-based PVC are grown. Homogeneous distribution of radii tends to produce high emission power. Therefore, the PVC should work at better efficiencies. Real QDs-based PVC are closer to a combination of Gaussians with characteristic radii allowing the dots to emit in different but not infinite range of the electromagnetic spectrum.

Acknowledgments

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Conflicts of Interest

The authors declare no conflict of interest.

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