Optimization of Solar Cells Efficiency, A Quantum Perspective

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Context

Photovoltaic (PV) production is the world's fastest growing energy technology.
The two major technological challenges that next-generation solar cells are facing are:

- **decreasing the price** to concurrence already established energy production sources and
- **increase the efficiency**. Durability, availability and toxicity are also important.

Quantum effects at the nano scale allow to design the electronic (and therefore optical) properties of **nanostructures** by changing materials, composition or geometries.
This allows PV devices with **optimized** key properties to maximize power conversion efficiency (theoretically beyond the Schokley-Queisser limit)

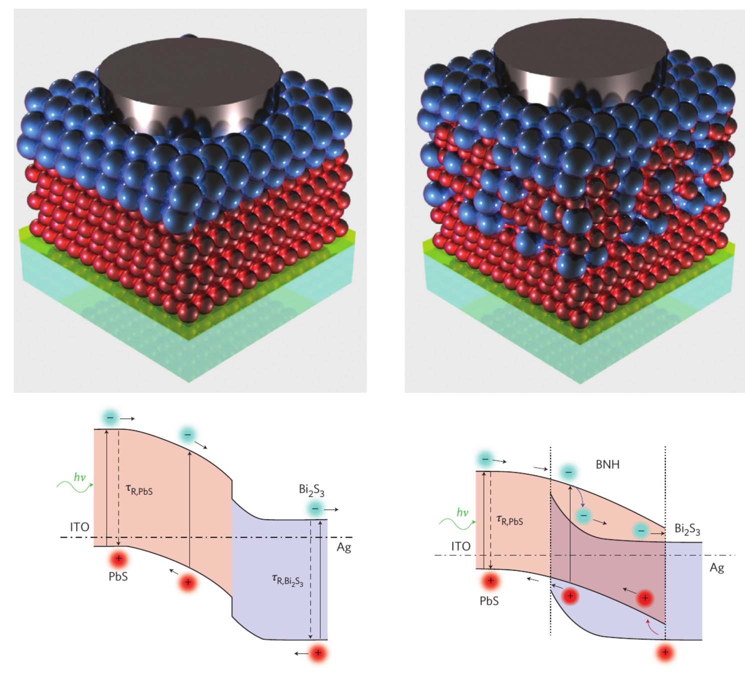
Objectives

- Calculate quantum nanostructures electronic properties accurately
- Evaluate optical and transport characteristics
- The method should be fast and general for an optimization approach

Goal: Estimate the power conversion efficiency of a solar cell from the quantum electronic properties

Choice of device

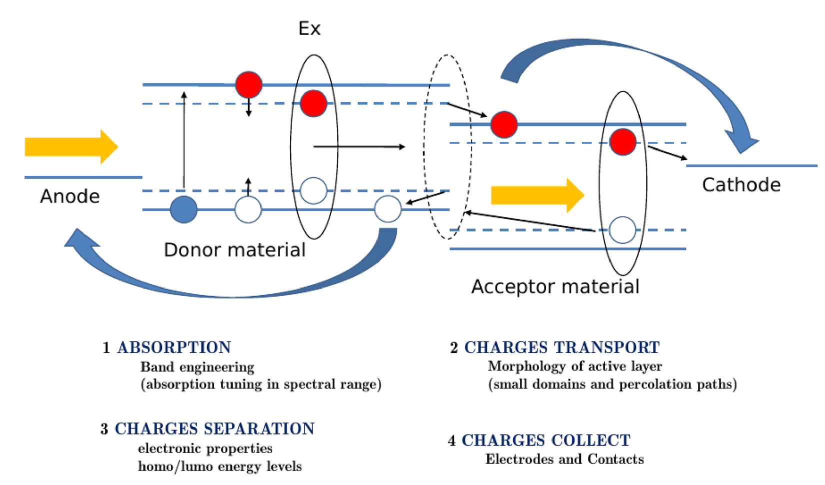
Almost all third generation solar cells use a quantum effect of some sort. The stronger (more promising) effects are for **Quantum Dots**. To increase the efficiency one can either increase the absorption or the transport and collect.



Improvements in charge transport when using bulk heterojunctions [1]

Numerous new PV technologies employ QDs but properties like flexibility, transparency and easy processing lead us to choose

Quantum Dots Hybrid Solar Cells



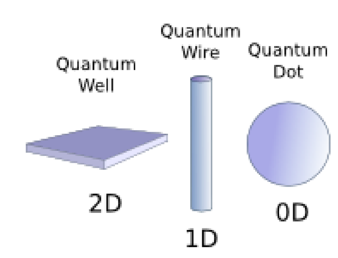
Hybrid solar cells, working principle and key electronic properties to influence

To validate our approach, we made spin-coated PMMA thin-films that incorporates quantum dots.
Those dots are (core)shell (CdSe)-CdS and -ZnS and massive PbS. Several sizes are available.

Methodology

Model a quantum structure

Quantum Wells (thin films in general), circular cross-section Quantum Wires and spherical Quantum Dot
Heterostructures and any kind of material if we know the effective masses and the potential profile



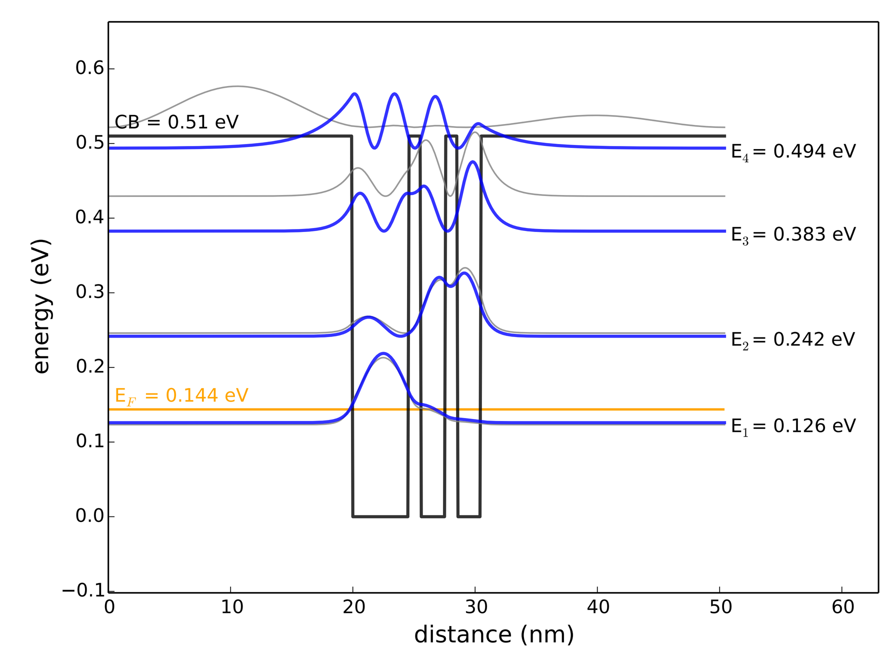
Resolve Schrödinger to get energy and wavefunctions

Effective mass approximation, the method is fast but overestimates the energy away from the band edge

Limitations for high confinement: Low-bandgap materials and small sizes

Correction: energy dependence of the effective mass

Accuracy improvement, we retrieve the precision of more computationally demanding methods



Effect of the nonparabolicity correction: InGaAs/AlInAs multiple quantum wells
We retrieve the results of 8-bands k·p methods

Study the electronic transitions

Electrostatic dipole model, the main results are matrix element, oscillator strength and plasma frequency
Corrections to make it appropriate to heterostructures

Evaluate Absorption and Transport characteristics

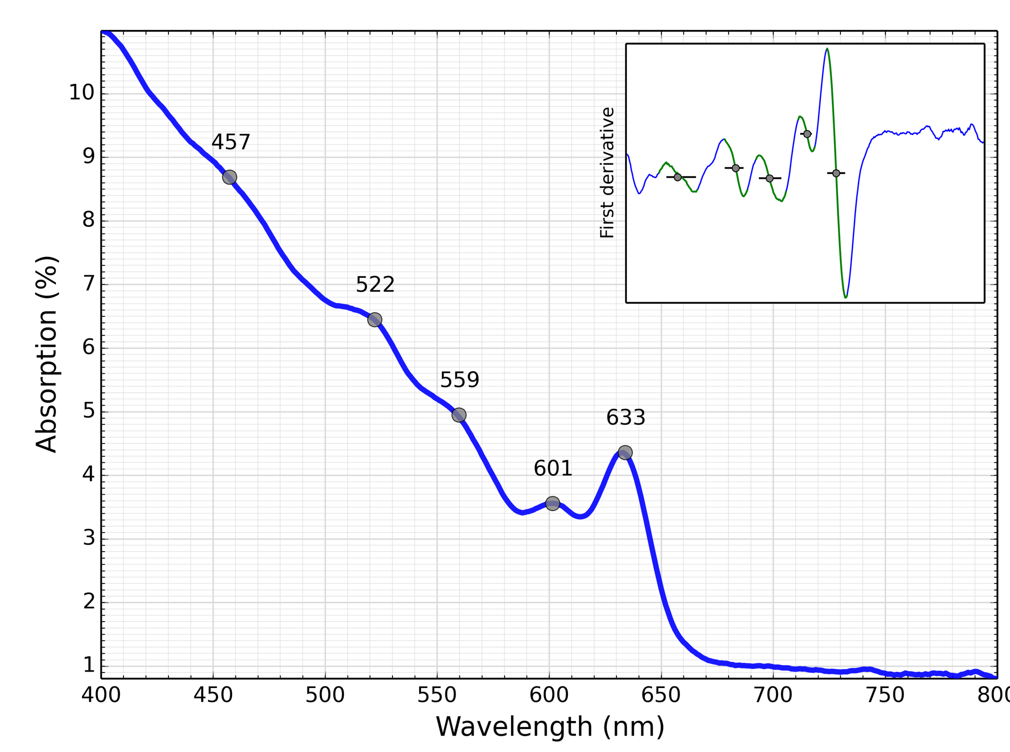
With the quasi-Fermi levels and levels population we calculate the absorption starting from the Fermi golden rule

Optimize charges absorption and transport thanks to confinement effects

Variational studies to find appropriate materials association, doping and sizes

Calculate the effective index in the nanostructure to use in our or others studies

Drude-Lorentz from transitions properties



Absorption spectrum of (core)shell (CdSe)CdS in PMMA thin film
Peak extraction procedure

Precisions on numerical methods

All of the code is implemented in **Python** except for the core calculation functions that are accelerated in Cython.

We use **finite difference** representation to construct our structures.

A **shooting method**, described in Harrison's book [2] is used for energy levels. It has been **improved** [3] and **reformulated** to resolve the three dimensionality (using symmetries of cylindrical and spherical geometries).

Accuracy limits come from the assumption that the curvature of the conduction (CB) and valence (VB) bands is parabolic. We use a **nonparabolicity correction** on the effective mass but as it is still not optimal we are currently testing a **new** formulation.

The correction to make the optical **parameters suitable for heterostructures** consists of normalizing the material parameters (m_i^* - ϵ_{r_i} - ...) by the form of the wavefunction $|\psi_i|^2$ for each electronic level i.

Current limitations

The main limitations are the **overestimation of the energies for low band-gap materials and small sizes** and the **sensibility to input parameters** (effective masses and potential) that are not

The optical transition elements are sensitive to the shape of the wavefunctions that are not independent of the finite structure geometry, especially the lengths of the calculation barriers.

When comparing numerical and experimental optical results quantitatively, attention has to be payed to dynamic mechanisms that affect the shape (amplitude and broadening) of the transitions phenomena

Perspectives

- Experimental validation of calculations → is the precision acceptable ?
- Simulation of an entire cell → the electrical part has to be developed
- Realisation and study of a QD-to-optimize/P3HT hybrid solar cell

References

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