Choice of Quantum Dots for Hybrid Solar Cells

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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.
- **increasing the efficiency**.
  Durability, availability and toxicity are also important.

Quantum effects at the nanoscale allow to design the electronic (and therefore optical) properties of **nanostructures** by changing materials, composition or geometries.

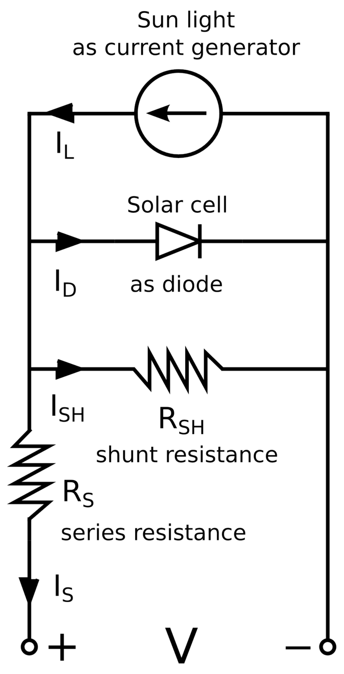
This allows PV devices with **optimized** key properties to maximize power conversion efficiency (theoretically beyond the Schokley-Queisser limit)

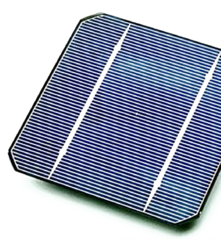
Objectives

- Evaluate the efficiency of hybrid solar cells depending on the materials
- Calculate quantum dots size-dependent properties
- Use data from the literature to evaluate different possibilities

Find optimal materials to obtain high efficiency hybrid solar cells

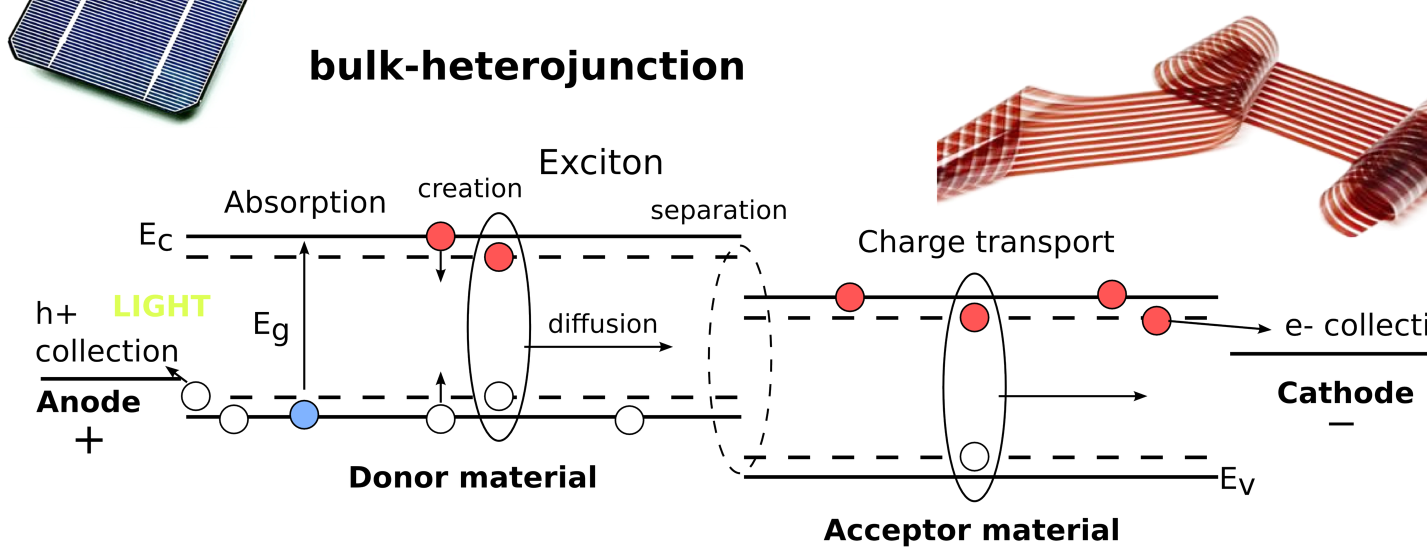
Hybrid Solar Cells





Solar cells
from "good old" silicium to **organic copolymers**

bulk-heterojunction



We choose hybrid organic solar cells because of the possibilities that are added with the use of **organic polymers**. The advantages that this new technology offers are:

- ease of processing, low-cost thin-film technologies (solution, roll-to-roll, printing, spraying, ...)
- low-cost, abundance and low-toxicity of copolymer materials
- transparency, flexibility, lightness, etc... that are interesting for innovative applications

But the efficiency is limited, the current record is 11.1% (25% for Si). This is why research is conducted towards the association with other materials such as **semiconductor nanostructures**.

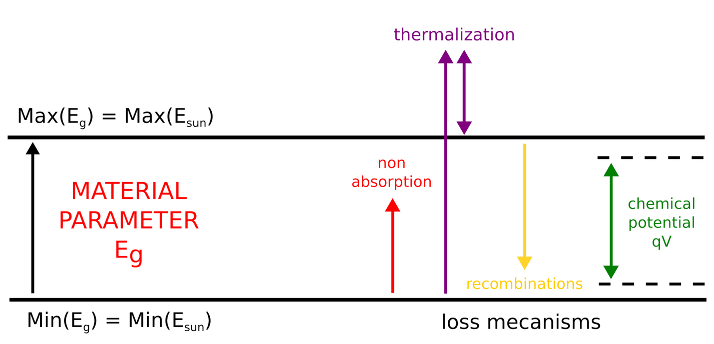
Solar cell Modeling

We use simple **detailed balance models** that evaluate the efficiency lowered by 4 main loss mechanisms.
The cell behaves like a diode.

Efficiency: $\eta = \frac{J_{sc} V_{oc} FF}{P_{in}}$

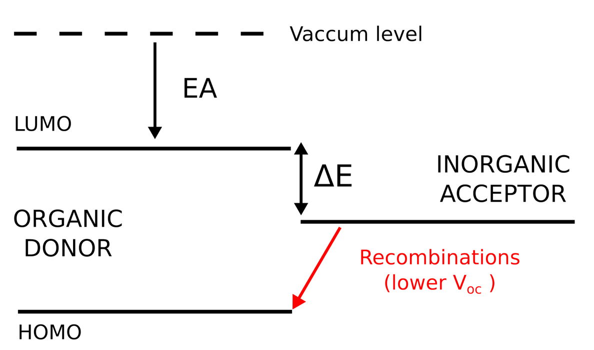
We calculate homogeneous and heterogeneous active layers.
No transport considerations

HOMOJUNCTION
Shockley-Queisser limit



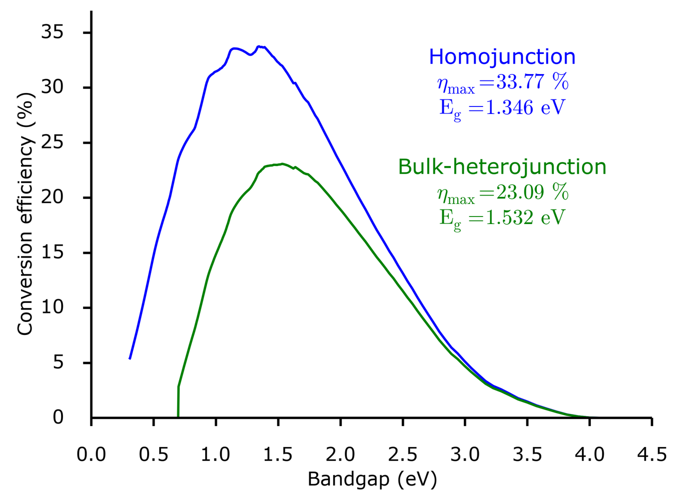
DETAILED BALANCE MODEL
Optimal Bandgap - E_g = 1.35 eV

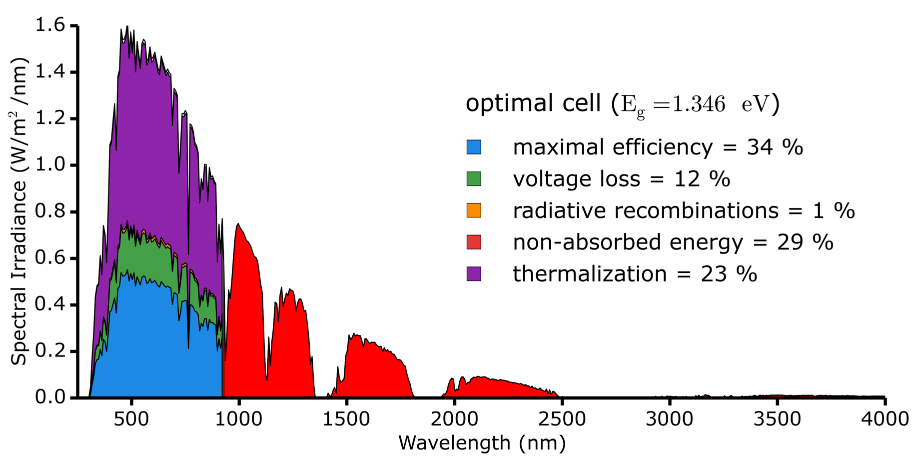
HYBRID HETEROJUNCTION

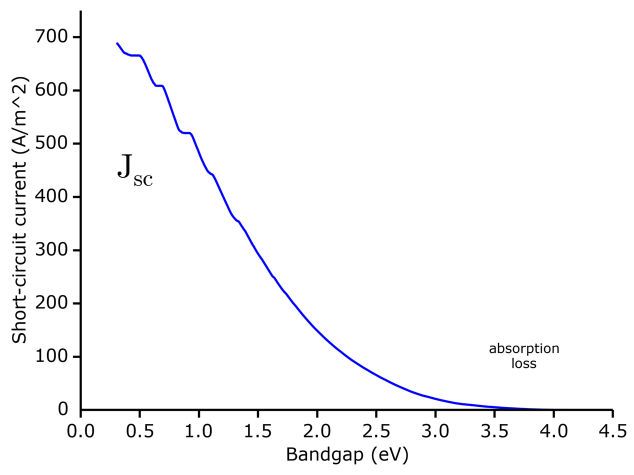


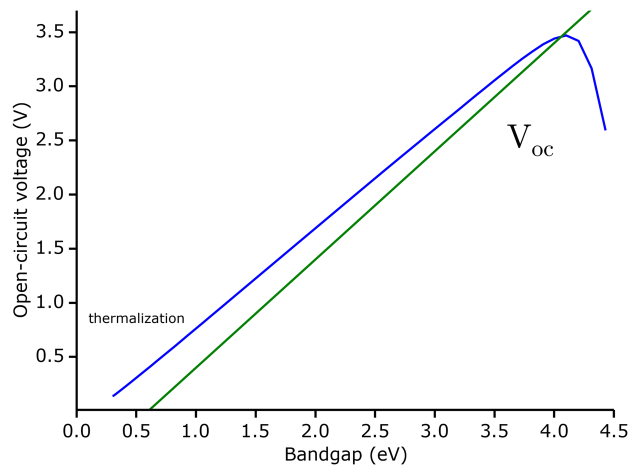
BAND ALIGNEMENT CONDITIONS
ΔE = E_b to minimize
EA to maximise

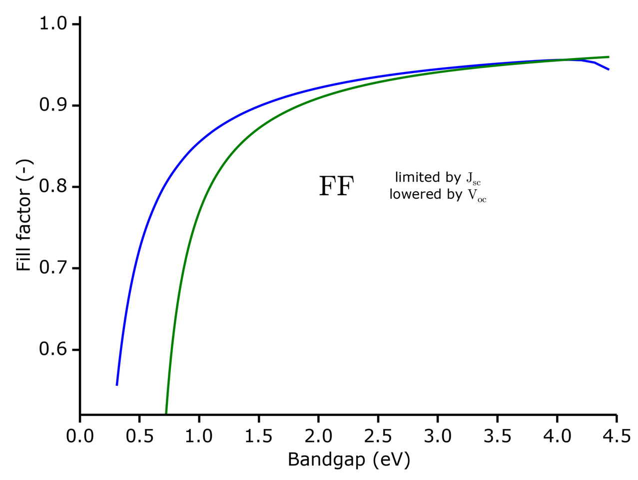
The **heterojunction model** is an extension of the homojunction model.
Empirical Voc impacted by recombinations at materials interface.
No extra-absorption in the acceptor material. **Only general conditions** for material selection.

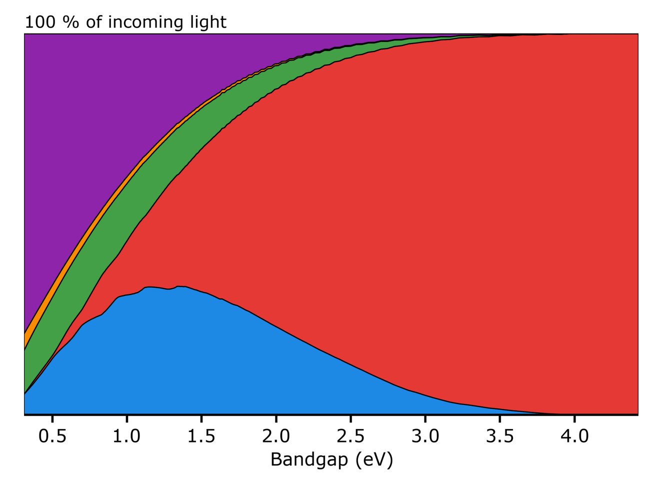






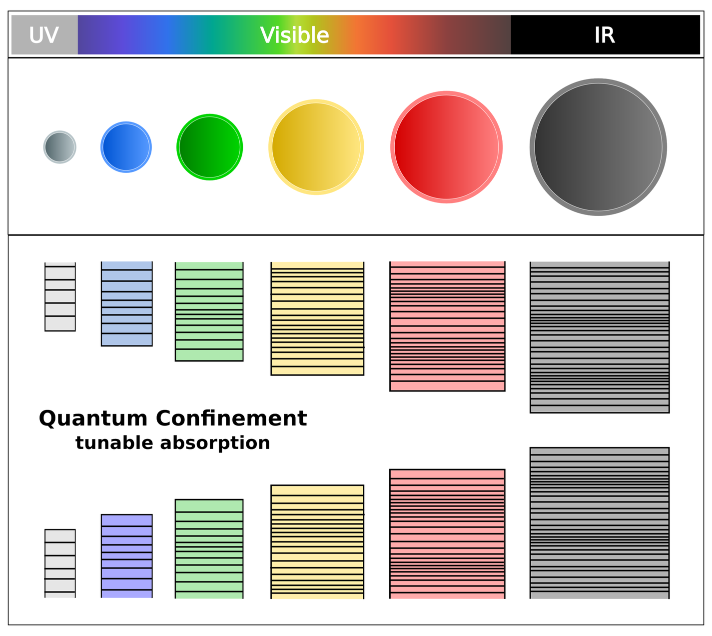






Quantum Dots

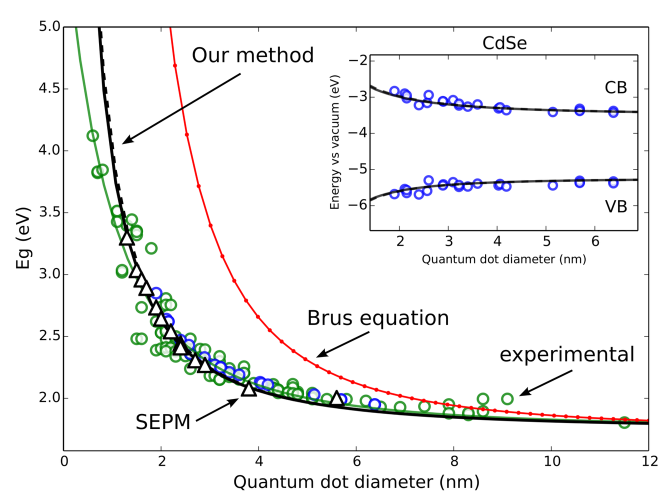
Quantum Dots (QDs) are nanostructures that are **confined** in the 3 dimensions of space. Those 0D structures behave like artificial atoms whose **properties can be tuned** with size.



Quantum dots are interesting to enhance absorption (higher dielectric permittivity).

QDs Calculations

Development of a simple, fast and precise **method to calculate energy levels** in quantum structures (wells, wires and dots)



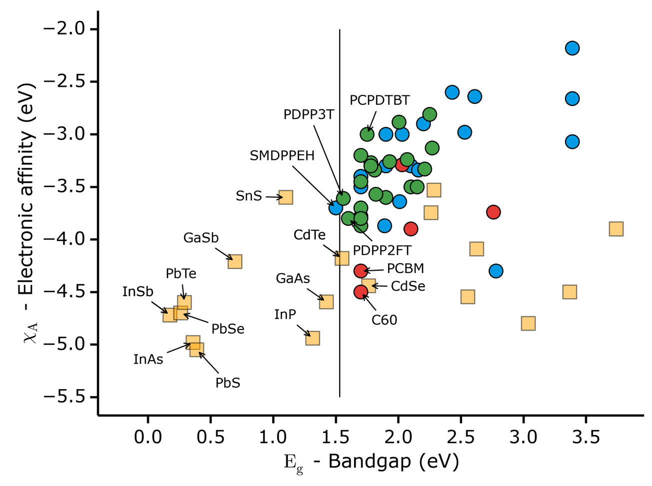
Calculations have been **tested** against extensive data from the literature.
We are now looking at the optical properties.

Perspectives

- Consider transport and optical phenomenas
- Take acceptor absorption into account
- Evaluate more materials and morphologies
- Realization of the hybrid SC active layer

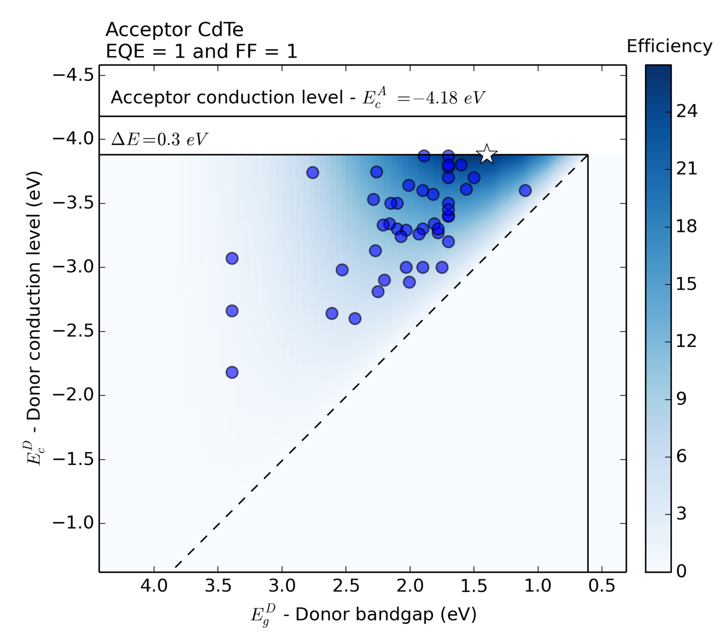
Materials Selection

Development of a **material database** to test our models and perform various material optimization approaches.



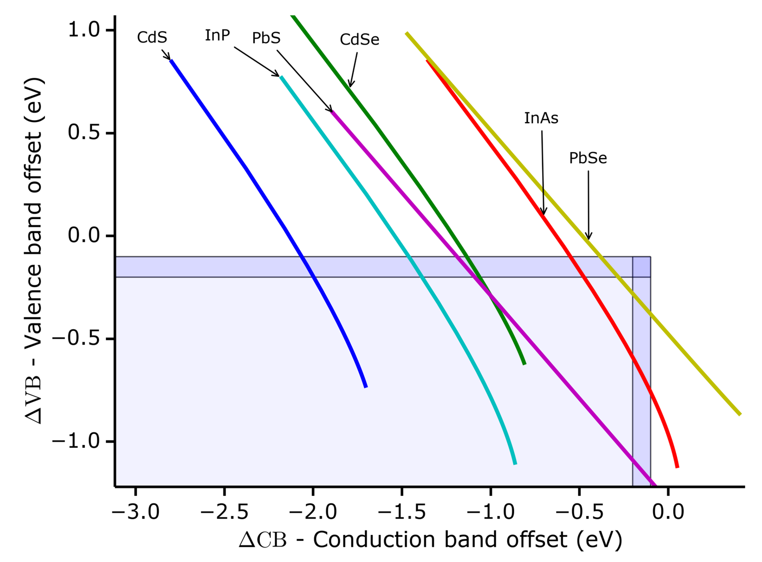
Search for a donor meeting heterojunction model criteria.
Lowest χ_A possible to minimize exciton binding energy and closest from the theoretical bandgap.

Particular acceptor.
Semiconductors have low electronic affinity...
Solution: Quantum confinement !



Donor	E_g (eV)	E_c (eV)	η (%)
P2	1.70	-3.87	24.63
PDPP2FT	1.60	-3.80	23.56
PDPP3F	1.70	-3.80	23.01
P1	1.70	-3.78	22.53
DCV4T	1.89	-3.87	22.12
SMDPPEH	1.50	-3.70	20.99
P3	1.70	-3.70	20.75
PDPP3T	1.56	-3.61	18.65
PSiFDTBT	1.82	-3.57	17.33
PCDTBT	1.90	-3.60	17.14

Search of ideal quantum dots by band alignment



Best acceptor for **PDPP2FT** = PbSe
(tested) QDs band-edges
for sizes between 1 and 20 nm.
Search window:
ΔCB et ΔVB between -0.1 and -0.2 eV or less.

References

[1] W. Shockley and H.J. Queisser. Detailed balance limit of efficiency of p-n junction solar cells. *J. Appl. Phys.*, 32(3), 1961.

[2] MC Scharber, D Wuhlbacher, M Koppe, and al. Design rules for donors in bulk-heterojunction solar cells - Towards 10 % energy-conversion efficiency. *Advanced Materials*, 18(6), 2006.

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Contact Informations

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