# The upper limit for the efficiency of organic solar cells: will organic photovoltaics be able to compete with traditional solar cells?

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**The current generation of photovoltaic solar cells (e.g. polycrystalline silicon cells) are too expensive to compete with the classical energy sources. Other materials for solar energy conversion are necessary to obtain a significant cost reduction. Therefore, organic solar cells are studied intensely during the last decade. However, in order to compete with the traditional inorganic cells, efficiencies of more than 10% are a necessity. Nowadays, efficiencies up to 5% are reached and the question about the limits for the attainable efficiency of organic cells arises. In this article, we calculate the upper limit for the efficiency of organic cells, and make realistic assumptions to predict realistic efficiencies obtainable in the near future. Ideal material characteristics are obtained from these calculations, giving an idea how the ideal organic solar cell should look like.**

Firstly, we consider a solar cell with one active material with a bandgap $E_g$. We make the following fundamental assumptions: (i) every photon with an energy $h\nu$ higher than the bandgap $E_g$ is absorbed. (ii) photons with an energy $h\nu$ lower than the bandgap $E_g$ are fully transmitted. (iii) every absorbed photon leads to a useful energy $E_g$. In this case, the maximum efficiency $\eta_{max}$ is given by:

$$\eta_{max} = \frac{E_g \int_{E_g}^{\infty} N(E)\,dE}{\int_{0}^{\infty} E\,N(E)\,dE}$$

with $N(E)$ the photon flux. For all our simulations, we use the AM 1.5 experimentally measured solar spectrum [1]. A maximum efficiency of 48.7 % is reached when $E_g$=1.14 eV, which is a well known result. However, producing suitable organic absorbers with such a low bandgap is a problem. When we take also into account a narrow absorption window (Figure 1 for definition of terms), characteristic for organic materials, the optimal bandgap shifts towards higher energies (Figure 2).
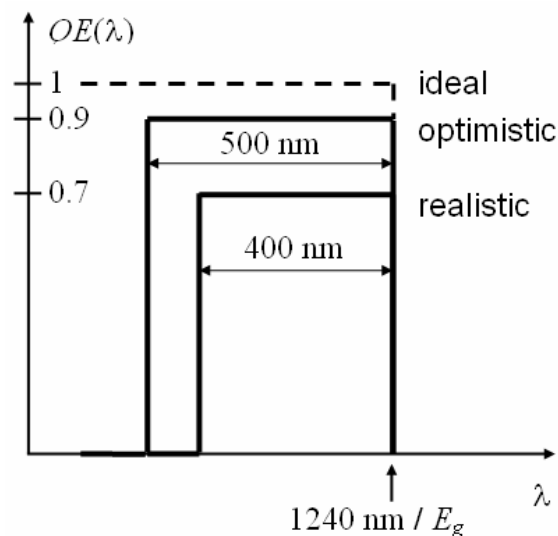


*Figure 1: Definition of terms: absorption window; ideal, optimistic and realistic scenario for absorption and quantum efficiency QE.*

For an absorption window of e.g. 300 nm, the optimal bandgap is 1.7 – 1.8 eV, which is in line with current organic absorbers. To estimate the maximum obtainable efficiency with the current state of technology, we assume the following realistic values, which are nowadays reached in organic photovoltaics. We assume an absorption window of 400 nm, a quantum efficiency $QE$ of 70%, a fill factor $FF$ of 65%, and a voltage factor $f$:

$$f = \frac{q \cdot V_{oc}}{E_g}$$

of 60%, with $V_{oc}$ the open circuit voltage. This results in a maximum attainable efficiency of 11 %. If we consider optimistic values, which however are credible to be achieved in the future, an efficiency of 22 % becomes possible (i.e. an absorption window of 500 nm, $QE$=90%, $FF$=80%, $f$=70%).

However, the active material in a bulk heterojunction solar cell consists not of one material, but of an interpenetrating network of an $n$-type (electron acceptor, e.g. fullerene derivatives) and a $p$-type (semi)conductor (electron donor, e.g. conjugated polymer), sandwiched between two electrodes with different work functions.
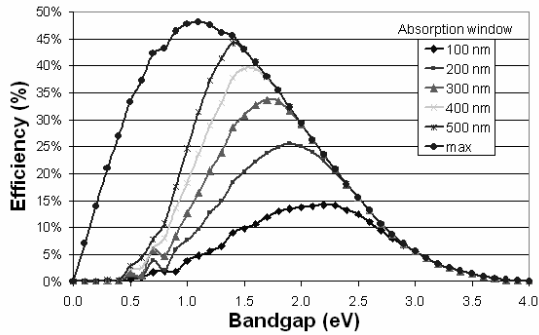
*Figure 2: The maximum efficiency as a function of the bandgap in a solar cell with one active material. A decrease of the absorption window leads to a shift (increase) in the optimal bandgap.*

For the simulation of an organic solar cell, the following assumptions are made (Figure 3 for definition of terms): (i) only one material absorbs light (usually, this is the *p*-type component) (ii) every photon with an energy $h\nu$ higher than the bandgap $E_{g,absorber}$ is absorbed, with the bandgap defined as the difference between the Lowest Unoccupied Molecular Orbital (LUMO) and the Highest Occupied Molecular Orbital (HOMO) of the absorber. (iii) not any photon with an energy $h\nu$ lower than the bandgap $E_{g,absorber}$ is absorbed. The distance between the HOMO of the donor, and the LUMO of the acceptor is considered as the thermodynamic limitation for the useful energy. This value is often called the interface bandgap $E_{g,i}$. We assume that (iv) every absorbed photon leads to a useful energy $E_{g,i}$.

One notices from Figure 4 that, with a full absorption window, the optimal bandgap of the absorber is again 1.1 eV. The highest efficiency is reached when the LUMO of the *p*-material is as close as possible to the LUMO of the *n*-material. This was expected, because the difference between the LUMO's corresponds with an energy loss of the absorbed photon.
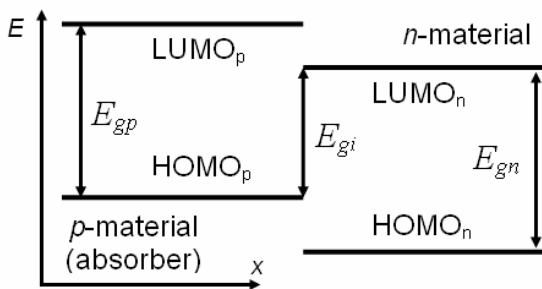


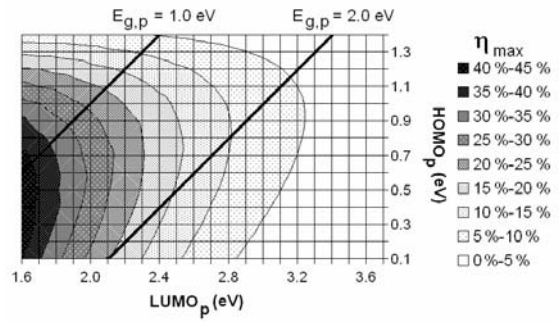*Figure 3: Definition of terms: absorber, HOMO and LUMO energy levels, interface bandgap.*



*Figure 4: $\eta_{max}$ as a function of the LUMO and the HOMO of the p-material for the case where the p-type material absorbs the light, and the n-type has a bandgap of 1.5 eV. The HOMO of the n-material is taken as a reference ($HOMO_n = 0$ eV). Two straight lines indicate where the bandgap of the p-material is 1.0 eV and 2.0 eV.*

In organic bulk heterojunction solar cells, light absorption does not lead immediately to free charge carriers, but an exciton is created. A necessary condition for efficient dissociation of the created excitons is that the difference between the LUMO's of the donor and acceptor is higher than the exciton binding energy. The value of the exciton binding energy in different materials is a subject of discussion, values between 0.1 eV and 2 eV are published [2]. For the simulations, we assume a difference of 0.2 eV between the LUMO's. This value was put forward as an empirical threshold necessary for exciton dissociation [3]. If we also take into account the realistic present and future values of the absorption window, *QE*, *FF* and *f* mentioned above, the maximum obtainable efficiency of organic bulk heterojunction solar cells is respectively 9.4 % and 19 %. This result indicates that organic solar cells have still a big efficiency potential, which can make it possible for them to compete with traditional inorganic solar cells.

ACKNOWLEDGEMENTS

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[3] *submitted*: B. Minnaert, M. Burgelman, Empirical study of the characteristics of current-state organic bulk heterojunction solar cells / Conference ECHOS 06, Paris, "The European Physical Journal - Applied Physics"