# A sunny future

## morphology and energy levels in organic solar cells.

PhD article

More than 3850 ZJ of power reaches the earth yearly. With the global energy consumption being only a fraction of that, sunlight would be an ideal source for energy production. How to get power from sunlight? Well, through solar cells of course! But as the efficiency is relatively low, the solar cell efficiency has to be increased to meet the daily consumption. A deeper understanding of the working principles of solar cells might bring all of us a sunny future!

### Me, myself and I

About nine years ago my first year at TU/e started. I came in as a seventeen-year-old guy, a bit too enthusiastic about going to university and not knowing about a future career and even whether Chemical Engineering was the correct bachelor program. Research, production or education; materials science, inorganic chemistry or something else? No clue yet… During my bachelor education, the (physical) chemistry directed courses were most interesting to me, so the (by then) master track in Molecular Engineering was the best option.

Some Japie members amongst you might be wondering… where do I know this guy from? Well, during my study I've been part of amongst others the IntroCie 2009, the XIth lustrum committee, and the Advisory Board. After all obligatory and some extra courses, choosing the graduation project was approaching. For me, the most obvious option was a project in the Molecular Materials and Nanosystems group. Ten months of inorganic, organic and electrochemistry later I had created an artificial leaf using an organic solar cell and earth-abundant catalysts. This was also the point at which I was offered the opportunity to start a PhD project in the same group a few months later.

### Organic solar cells

Apart from chemistry, physics always has been an important and interesting scientific area to me. As Robert

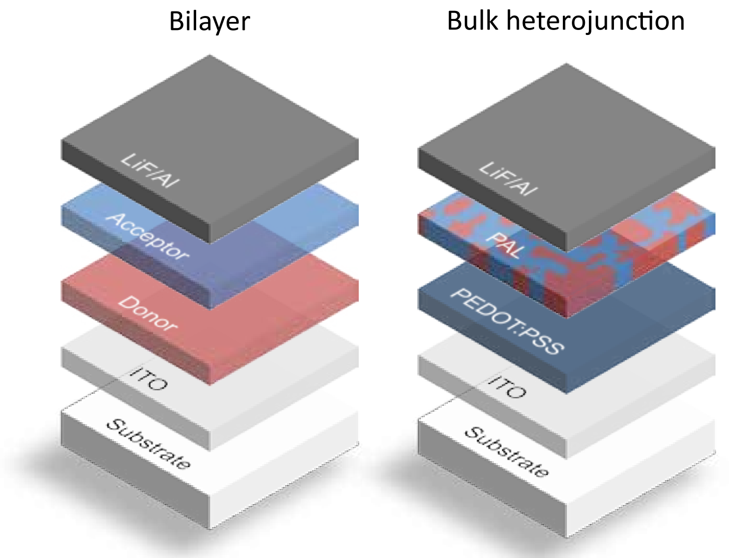

*Figure 1: Schematic representation of a bilayer and a bulk heterogeneous solar cell*

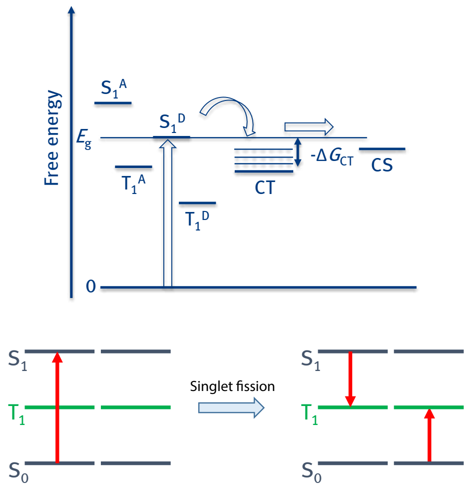

*Figure 2:*
*Top diagram: State-diagram picture with energy levels*
*Bottom image: state-diagram for singlet fission*

*Photo by Bart van Overbeeke*

Wilhelm Bunsen (yes, the one who didn't invent the Bunsen burner but only upgraded a known design from Michael Faraday) already mentioned in the 19th century: "Ein Chemiker, der kein Physiker ist, ist überhaupt gar nichts." Or, in English: "A chemist who is not a physicist, is nothing at all." Taking that and my love for both chemistry and physics in mind, physical organic chemistry would provide the perfect combination. The moment a group of physicists don't notice you are not a physicist but a chemist, I think you can say one of my life goals had been achieved!

In my PhD project, I work on organic solar cells. In the 1950s and 1960s, the first organic solar cells were shown in literature. Organic solar cells have relatively laboratory efficiencies of 10-15%, although, they have many promising properties such as low fabrication costs, flexibility, and semitransparency. Imagine a window that can power your phone or roof tiles, which can generate power themselves.

Figure 1 shows two different architectures of organic solar cells: the bilayer solar cell and bulk heterojunction solar cell. In both architectures of solar cells, an active layer is sandwiched between two selective contacts of which one is transparent. This active layer consists of two materials: an electron donor and an electron acceptor material, which have different energy levels. Typical examples of the electron donor are small molecules like pentacene and polymers such as P3HT, while the commonly used electron acceptor is a fullerene derivative.

When light hits the solar cell, it's absorbed by the active layer and a singlet excited state is generated (or, one electron is excited from the highest occupied molecular orbital to the lowest unoccupied molecular orbital). At the interface of the electron donor and electron acceptor, a charge-transfer state will spontaneously be generated by transfer from the generated singlet state. The charge-transfer state can either relax thermally or electronically, but also separate into a hole on the donor and an electron on the acceptor.(1) The latter process is the process that will generate the current from the solar cell.

## Singlet fission

A striking way to increase the current generated by the solar cell is via so-called singlet fission. Singlet fission is a process in which one photon can be converted into two electrons by converting one singlet state into two triplet states. Say what? Yes, instead of one electron per photon, now two electrons per photon can be generated, both with lower energies as shown in figure 2. One way to show this effect is by measuring the external quantum efficiency, which is a measure of the number of electrons generated per incoming photon. When this EQE is over 100%, singlet fission plays a role.(2)

To study the influence of the energy levels of the fullerene on the performance and EQE of the solar cell, we have used different electron acceptor materials combined with pentacene as an electron donor. When the reduction energy of the fullerene is more negative, the generated voltage increases while the current and EQE clearly decrease. The threshold for this effect is when the charge-transfer state is equal to the triplet state of pentacene. This gives indirect evidence that the current generation has to go via the triplet state and that singlet fission plays a role in these solar cells.

## HOMO energy levels

The charge-transfer state plays an important role as it, for example, determines the voltage delivered by the solar cell.(3) The energy level of the charge-transfer state depends for example also on the HOMO energy of the electron donor material. However, what is the 'correct' HOMO energy level of the material? What is the best way to determine it and how are for example measurements performed with cyclic voltammetry, ultraviolet photoelectron spectroscopy and the open-circuit potential of the solar cell related? In the next part of my project I hope to find an answer to this question.

WRITTEN BY:

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