# SKM-Symposium Elementary Processes in Organic Photovoltaics (SKM-SYOP)

jointly organized by
the Chemical and Polymer Physics Division (CPP),
the Thin Films Division (DS), and
the Semiconductor Physics Division (HL)

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In spite of intensive research, the photovoltaic properties of organic solar cells are not yet completely understood. Current open questions include the dynamics of excited states as well as the generation and extraction of free carriers in organic multi-component systems. Recent research has shown that these processes are closely connected to the multi-scale architecture of organic solar cells. This includes the electronic structure of the molecules and polymers used, the intermolecular order and, finally, the supramolecular arrangement in the device. Real improvements in device performance can be achieved through a better understanding of these elementary processes, requiring a close exchange between scientists in different fields of research. The symposium "Elementary Processes in Organic Photovoltaics" will create a forum for scientists involved in the design and structure of organic thin films, the nature and dynamics of excited states, and the generation of free carriers as well as full device simulations.

## Overview of Invited Talks and Sessions

(lecture room TRE Math)

### Invited Talks

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| SKM-SYOP 1.1 | Mon | 10:30–11:00 | TRE Ma | **Charge separation in organic solar cells and the principle of detailed balance** — •Uwe Rau, Thomas Kirchartz |
| SKM-SYOP 1.2 | Mon | 11:00–11:30 | TRE Ma | **Three-Dimensional Nanoscale Organization of Bulk Heterojunction Polymer Solar Cells** — •Joachim Loos |
| SKM-SYOP 1.3 | Mon | 11:30–12:00 | TRE Ma | **Reliable prediction of charge transfer excitations using optimally tuned range-separated hybrid functionals** — •Leeor Kronik |
| SKM-SYOP 1.4 | Mon | 12:00–12:30 | TRE Ma | **Charge separation and recombination in organic solar cells** — •James Durrant |
| SKM-SYOP 1.5 | Mon | 12:30–13:00 | TRE Ma | **Efficient and stable organic vacuum deposited p-i-n-type tandem solar cells** — •Martin Pfeiffer |

### Sessions

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| SKM-SYOP 1.1–1.5 | Mon | 10:30–13:00 | TRE Ma | **Elementary Processes in Organic Photovoltaics** |

# SKM-SYOP 1: Elementary Processes in Organic Photovoltaics

Time: Monday 10:30–13:00 Location: TRE Ma

**Invited Talk** SKM-SYOP 1.1 Mon 10:30 TRE Ma
**Charge separation in organic solar cells and the principle of detailed balance** — •Uwe Rau[1] and Thomas Kirchartz[2] — [1]IEK5-Photovoltaics, Forschungszentrum Jülich, Germany — [2]Experimental Solid State Physics, Blackett Laboratory of Physics, Imperial College London, UK

The invention of the solar cell as an electro-optical power device dates back to the year 1954. In 1961, Shockley and Queisser derived the maximum conversion efficiency of an ideal pn-junction solar cell by applying the principle of detailed balance. This principle, known since the years 1924/25, is strictly valid only close to thermal equilibrium. Despite of this restriction, application of this principle to solar cells under illumination, i.e. in a non-equilibrium situation, is commonly accepted and successfully used even for the analysis of non-ideal solar cells. During the last two decades, new photovoltaic technologies like dye sensitized or organic solar cells have emerged from laboratories. The large difference of organic semiconductors to their inorganic counterparts challenges our general understanding of solar cells. The present contribution will start from the fundamentals of photovoltaic energy conversion and discuss the principles that are common to all these devices. In a next step, a general approach based on the principle of detailed balance is introduced that allows us to describe organic and inorganic solar cells and to highlight their different working principles. These differences have immediate consequences on the limitations, the practical design and the technical realization of the various types of devices.

**Invited Talk** SKM-SYOP 1.2 Mon 11:00 TRE Ma
**Three-Dimensional Nanoscale Organization of Bulk Heterojunction Polymer Solar Cells** — •Joachim Loos — University of Glasgow, School of Physics and Astronomy, Glasgow, Scotland, UK

Polymer and hybrid solar cells have the potential to become one of the leading technology of the 21st century in conversion of sun light to electrical energy because their ease processing from solution producing printable devices in a roll-to-roll fashion with high speed and low cost. The performance of such devices critically depends on the nanoscale organization of the photoactive layer, which is composed of at least two functional materials, the electron donor and the electron acceptor forming a so-called bulk heterojunction; however, control of its volume morphology still is a challenge. In this context, advanced analytical tools are required that are able to provide information on the local volume morphology of the photoactive layer with nanometer resolution. In this contribution we introduce electron tomography as the technique being able to explore the 3D morphology or polymer and hybrid solar cells and critically discuss first results achieved.

**Invited Talk** SKM-SYOP 1.3 Mon 11:30 TRE Ma
**Reliable prediction of charge transfer excitations using optimally tuned range-separated hybrid functionals** — •Leeor Kronik — Weizmann Institute of Science, Rehovoth, Israel

Charge transfer excitations are an essential concept in organic photovoltaics. Typically, electron excitations are well-described from first principles using time-dependent density functional theory (DFT). However, this is not the case for charge transfer excitations, which are very poorly described by all widely used approximations within time-dependent DFT.

Here, we overcome this difficulty by presenting a broadly-applicable, non-empirical first-principles approach based on using a range-separated hybrid functional within the generalized Kohn-Sham approach to time-dependent DFT. Its key element is the optimal choice of a range-separation parameter such that Koopmans' theorem is obeyed as closely as possible. We explain the physics behind this approach and demonstrate its validity, accuracy, and advantages for determining charge transfer excitation energies. Additionally, we show that the same approach can be used for predicting fundamental gaps of finite objects directly from generalized Kohn-Sham DFT eigenvalues.

* Work performed in collaboration with T. Stein and R. Baer, Hebrew University, Jerusalem

**Invited Talk** SKM-SYOP 1.4 Mon 12:00 TRE Ma
**Charge separation and recombination in organic solar cells** — •James Durrant — Imperial College London

My lecture will focus on charge separation and recombination in polymer / fullerene solar cells. The talk will be based around transient optical and optoelectronic studies of yields and lifetimes of charge carriers in blend films and solar cells. Comparative studies will be presented of different materials systems, including over 20 different polymers. On the basis of these data, I will address the parameters which influencing charge separation and recombination, including the roles of interfacial energetics, interface structure and blend nanomorphology and macroscopic electric fields and how these processes impact upon device performance.

**Invited Talk** SKM-SYOP 1.5 Mon 12:30 TRE Ma
**Efficient and stable organic vacuum deposited p-i-n-type tandem solar cells** — •Martin Pfeiffer — Heliatek GmbH, Dresden, Germany

We report on latest progress in the field of p-i-n type tandem solar cells. An efficiency of 8.3% on an active area of 1cm* has been confirmed by Fraunhofer ISE for a tandem cell where both photoactive layers are based on bulk-heterojunctions comprising a donor-type oligomer co-deposited with fullerene C60. We discuss the remaining loss factors in the present system and the way towards further optimization. Moreover, we show that p-i-n type tandem solar cells can be extremely stable: Extrapolated lifetimes corresponding to more than twenty years of illumination have been achieved for cells with an initial efficiency of 6%. Moreover, we report on efficient modules with integrated series interconnection. Finally, we show that high efficiencies (above 6% on 1cm^2) and lifetimes (several thousand hours both in a light-soaking test and when stored at 85°C) can be achieved for p-i-n tandem cells prepared on PET foil.