



## Theoretical and experimental pathways to a new efficiency regime for molecular solar cells

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In the first part, I will present several pathways to organic solar cells with power conversion efficiencies in excess of 20%. A model based on Marcus theory of electronic transfer that also considers exciton generation by both the electron donor and electron acceptor is used to show how reduction of the reorganization energies can lead to substantial efficiency gains.

We introduce the dielectric constant as a central parameter for efficient solar cells. We analyze how the dielectric constant influences every fundamental step in OPV. We analyze and model the case of the 2009 world record PTB7:[70]PCBM cell of 7.4%, using a drift-diffusion model. Based on the model and based on the fact that the exciton binding energy diminishes with increasing dielectric constant of the medium, we find that efficiencies of more than 20% are within reach upon increasing the dielectric constant  $\epsilon_r$  of the material to 10.

A completely different approach towards high efficiency PV is based on photon management. We report on our recent discovery of efficient broadband near-IR light up-conversion. Photon upconversion of the (near)infrared (NIR) photons is a promising way to overpass the Shockley-Queisser limit that sets up the maximal efficiency of 32% to a single junction solar cell. However, the practical applicability of the most efficient upconversion materials known to date at moderate light intensities (i.e. below 1000 Suns) is limited by the extremely weak and narrow-band (N)IR absorption. Here we, inspired by a natural design of photosynthetic complexes, introduce a novel concept of an upconversion material in which an organic (N)IR dye is used as an antenna for  $\beta$ -NaYF<sub>4</sub>:Yb,Er nanoparticles (NPs) where the upconversion occurs. The overall upconversion efficiency of the dye-sensitized NPs is dramatically enhanced (by a factor of  $\sim 3300$ ) as a result of increased absorptivity and overall broadening of the absorption spectrum of the upconverter. The proposed concept can be readily extended to cover any desired part of the solar spectrum by applying a set of dye molecules with overlapping absorption spectra acting as an extremely broadband antenna system, connected to a suitable upconverter.