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

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In the first part, we present three different theoretical approaches to identify pathways to organic solar cells with power conversion efficiencies in excess of 20%. We take off after reasoning why the Shockley-Queisser limit is applicable to OPV. A radiation limit for organic solar cells is introduced that elucidates the role of charge-transfer (CT) state absorption. Provided this CT action is either sufficiently weak or present in its maximized form throughout the active layer material, organic solar cells can be as efficient as their inorganic counterparts.

Next, 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.

Third, 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 inceasing dielectric constant of the medium, we find that efficiencies of more than 20% are within reach upon increasing the dielectric constant $\varepsilon_r$ of the material to 10 (Figure 1).

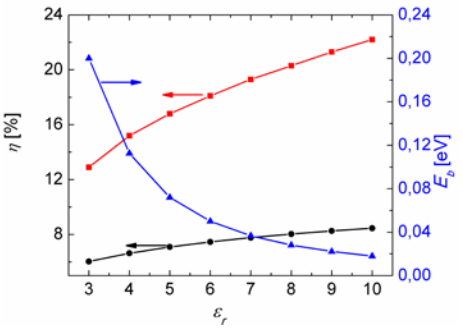


*Fig1: (black line) $\eta_{(PTB7:[70]PCBM)}$ as function of $\varepsilon$; (blue line) exciton binding energy $E_b$ as function of ;(red line) $\eta$ of OPV with $E_b$ optimized for each value of $\varepsilon$.*

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 β-NaYF4:Yb,Er nanoparticles (NPs) where the upconversion occurs. The overall upconversion efficiency of the dye-sensitized NPs is dramatically enhanced (by a factor of ~3300; see Fig. 2) 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.

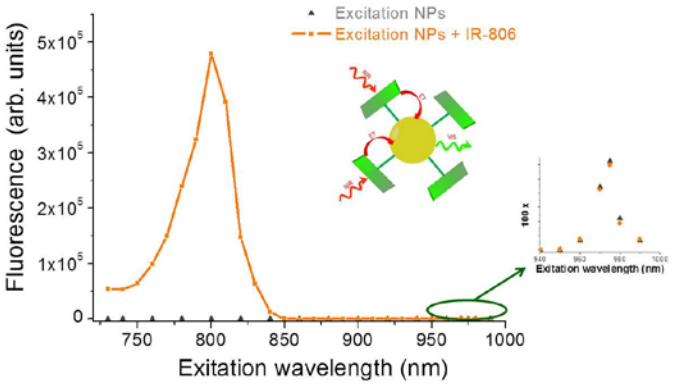


*Fig 2. Upconversion action spectrum of IR-806-coated β-NaYF4:Yb,Er NPs (orange line). Insets: cartoon of dye-coated NPs and amplified action spectrum showing the original NP upconversion.*