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## **Energy Losses in Small-Molecule Organic Photovoltaics**

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After intense research and development organic solar cells have matured among the family of thin-film photovoltaic technologies. On the laboratory scale they reach power conversion efficiencies in excess of 10%. Together with other attractive features, like transparency or the compatibility with low-cost, large area processing, they open reasonable perspectives for their commercialization. However, in order to close the gap to established inorganic technologies, primarily crystalline silicon, the fundamental understanding of loss processes has to be improved.

First and foremost, this concerns the energy loss between the optical gap for light absorption and the open-circuit voltage of the cell. In this Research News the scientific background for the different mechanisms of energy losses in organic photovoltaic cells together with current approaches toward their reduction are presented.

## 1. Introduction

Organic photovoltaics (OPVs) have made tremendous progress over the last three decades. Starting with a power conversion efficiency (PCE) of only 1% in the first OPV cell using a heterojunction concept [1], this value has meanwhile exceeded 10% [2] and has encouraged the vision of low-cost, large-area applications of OPVs [3]. Nevertheless, they still lag behind crystalline inorganic solar cells based on silicon, which are presently dominating the market for photovoltaic (PV) applications [4]. Moreover, with the rapidly progressing hybrid organic-inorganic perovskite solar cells a very attractive candidate for solution processible PV technology has recently appeared as well [5].

Comparing the different technologies in terms of PCE, which is specified as the product of the short-circuit current density  $j_{SC}$ , the open-circuit voltage  $V_{OC}$  and the fill factor  $FF$  divided by the incoming light intensity under standard AM 1.5G illumination conditions, OPVs can well compete with their inorganic counterparts in terms of  $j_{SC}$  or, more precisely, the external quantum efficiency and also with minor trade-off in  $FF$ , but clearly suffer from lower  $V_{OC}$  at a given energy gap  $E_g$  of the light absorbing material. While this so-called bandgap-voltage offset can be as low as 0.3-0.4 eV in Si and GaAs [6] and only a little larger in perovskite cells [7], OPV cells exhibit energy losses of at least 0.6 eV – in many cases, however, this offset can approach and even exceed 1 eV [8]. This is currently one of the main bottlenecks toward making OPVs competitive with inorganic PV cells.

In this Research News we provide the required background information on the appearance of energy losses in OPV cells, by which we mean the difference between the equivalent of the optical gap and the measured open-circuit voltage that is frequently also denoted as voltage loss, and discuss recent progress toward better understanding their origin and strategies to reduce them. To keep focused, we will mainly address small molecules as active organic semiconductors, which are being processed into thin films by vacuum deposition techniques. Compared to frequently studied  $\pi$ -conjugated polymers, the synthesis of small molecules is more reproducible. Moreover, a rigorous purification of small molecules is easier, which gives the opportunity to reproducibly investigate well-defined systems. The application of vacuum deposition techniques prevents the use of solvents, which as a third component in wet chemical processing can strongly influence the morphology [9]. Thus, active layers of small molecules prepared by vacuum deposition methods mark a well-controlled model system for fundamental studies such as the origin of energy losses in OPV devices. However, we expect that most of the findings can be transferred to solution-processed OPVs as well, which have considerably higher complexity in terms of local morphology and phase behavior.

## 2. Excitonic organic solar cells

In order to properly address energy losses in OPVs it is useful to look at their working principles in more detail (see also [10]). Conceptually, they differ from inorganic cells by their quasi-Fermi-level splitting being inherent to the photo-generation of charge carriers as well as by the excitonic nature of photoexcitations in organic semiconductors. Thus, the primarily formed species after absorption of a photon in the absorber material (with an optical gap  $E_g$ ) is a strongly bound electron-hole pair residing on one and the same molecule, i.e. a molecular exciton. With exciton binding energies of the order of 0.5 eV it is clear that this state cannot simply be dissociated by thermal energy as in inorganic PV materials. It requires a heterojunction between two materials, a donor (D) and an acceptor (A), with different ionization energies and electron affinities, so that an electron transfer from D to A can occur (see **Figure 1(a)**) or, vice versa, a hole transfer from A to D, if the photon is originally absorbed in the acceptor material. The electron on A and the hole on D are still Coulombically bound and form a so-called charge transfer (CT) exciton, which can either be separated into freely moving charge carriers or recombine at the D-A interface releasing its energy  $E_{CT}$  by emitting a photon or in a non-radiative process. As a consequence, the morphology of the active layers and the interface energetics will be of outmost importance for the PCE. Those carriers that do not recombine (either geminately at the D-A interface, if they stem from the same exciton, or non-geminately, if they recombine after splitting of the exciton on their way to the electrodes) can be extracted from the solar cell and deliver power to an external load. Thereby,  $q \cdot V_{OC}$  (with  $q$  being the elementary charge) is an upper limit for the work delivered per absorbed photon.

According to this scenario, there are two main steps, where energy losses occur: (1) in the charge transfer process between  $E_g$  and  $E_{CT}$  to form the CT state, and, (2) in the process of charge separation and extraction between  $E_{CT}$  and  $V_{OC}$ . Thus,  $V_{OC}$  can be written as:

$$q \cdot V_{OC} = E_g - \Delta E_{CT} - \Delta E_{rec} \quad (1)$$

with  $\Delta E_{CT}$  being the so-called driving force for the formation of the CT state and  $\Delta E_{rec}$  the recombination loss in its dissociation and conversion to free carriers performing work in the external circuit. Note that, strictly speaking, at  $V_{OC}$  the PV cell does not deliver any power at all, but it is generally accepted to take this value instead of the voltage at the maximum power point.

Due to their different physical origin it is common to treat both loss terms separately. In particular, the following expression is frequently used to quantify recombination losses only:

$$q \cdot V_{OC} = E_{CT} - \Delta E_{rec} \quad (2)$$

Following the approach by Shockley and Queisser (SQ) [11], the schematic absorption spectrum displayed in Figure 1(b) can be used to calculate an upper limit for the PCE of an excitonic solar cell [12, 13]. Therein, the single step profile with an onset at the energy gap  $E_g$  (which has to be identified with the optical gap of the organic semiconductor having the smaller gap) and unity absorbance  $\alpha_g \equiv 1$  has to be extended by a second step corresponding to the CT state, which is characterized by two parameters  $E_{CT}$  and  $\alpha_{CT}$ .  $E_{CT}$  is lower than  $E_g$  by the driving force  $\Delta E_{CT}$  and the absorption strength  $\alpha_{CT}$  typically is of the order of  $10^{-3}$  times the fundamental absorption across the optical gap. It is interesting to note that while the presence of the CT state in the subgap region has very little effect on the current  $j_{SC}$ , it has a significant impact on the voltage  $V_{OC}$ , as will be shown below.

Both parameters,  $E_{CT}$  and  $\alpha_{CT}$ , have been used as variable input for calculating the modified SQ limit of an excitonic solar cell [13]. Figures 1(c) & (d) show the results for the PCE and the  $V_{OC}$  at different combinations of  $\Delta E_{CT}$  and  $\alpha_{CT}$ . As expected, the PCE as function of  $E_g$  (Figure 1(c)) decreases with increasing  $\Delta E_{CT}$  and at the same time the position of its maximum is moving to slightly larger values. Importantly,  $\alpha_{CT}$  has a pronounced effect on both the PCE and  $V_{OC}$  (Figure 1(d)). Especially, if  $\alpha_{CT}$  is lowered from the typical value of  $10^{-3}$  found in a bulk heterojunction, i.e. in a co-evaporated equimolar D:A mixture, toward extremely small values,  $V_{OC}$  increases by a few tenths of an eV and can even exceed  $E_{CT}$  and reach the value predicted by SQ theory for the given gap. Note that the dramatic increase in PCE for  $\alpha_{CT}$  approaching 1 is due to the effect of a reduced energy gap  $E_g = E_{CT}$ , approaching the optimum gap of the SQ limit in this case.

While these simulations can provide an upper limit for the PCE of OPVs and nicely demonstrate the importance of both the energy level offsets at the D-A interface as well as the absorption strength of the resulting CT state for the total energy loss, they miss one important ingredient, viz. the presence of non-radiative recombination. Thus, the recombination loss term ( $\Delta E_{rec}$ ) in Equation (2) has to be extended to account for both contributions, leading to the following expression for  $V_{OC}$ :

$$q \cdot V_{OC} = E_{CT} - \Delta E_{rec}^r - \Delta E_{rec}^{nr} \quad (3)$$

As shown in the literature, the radiative loss term ( $\Delta E_{rec}^r$ ) depends logarithmically on the absorption strength  $\alpha_{CT}$  of the CT state, and the non-radiative loss ( $\Delta E_{rec}^{nr}$ ) can be written as  $-\ln(\eta_{EL})$  with  $\eta_{EL}$  being the electroluminescence (EL) quantum efficiency for light emission from CT states [14]. Actually, as several authors have pointed out, because of the extremely

low values of  $\eta_{EL}$  of the order of  $10^{-6}$  (as compared to  $10^{-3}$ - $10^{-2}$  in GaAs, Si or perovskites) the non-radiative loss term is the dominant one in OPVs [7, 15]. Though the microscopic origin for the low EL quantum efficiencies has not been clarified yet, empirically, a linear relationship  $q \cdot V_{OC} = E_{CT} - 0.6 \text{ eV}$  was obtained over a wide range of energies covered by both polymeric as well as molecular materials [14, 16, 17]. Compared to the bandgap-voltage offset in Si or GaAs solar cells (0.3-0.4 eV) the recombination loss between  $V_{OC}$  and  $E_{CT}$  in OPVs is significantly higher. Moreover, one has to be aware that in many cases an additional loss comes from the fact that the driving force  $\Delta E_{CT}$  is non-negligible. Therefore, other authors have considered the performance of OPVs with respect to the total energy loss, i.e.  $E_{loss}^{tot} = E_g - q \cdot V_{OC}$ . However, they arrived at a similar conclusion that at least 0.6 eV energy losses are involved in efficient charge generation in OPVs [18, 19].

Beyond the simple model presented above, more complex and realistic models for the density of CT and transport states have been applied (see e.g. [20]). In particular, the recent work by Burke et al. [21] gives an expression that relates  $V_{OC}$  losses to the degree of disorder of CT states, their volume fraction of the cell and their lifetime. Taking typical values for these parameters the authors could well reproduce energy losses in the above mentioned range. Moreover, these and other authors have pointed out that the CT manifold can be more complex than one single band due to the coexistence of mixed and aggregated phases, which may be amorphous or crystalline as well [22, 23, 24]. This can have multiple consequences, such as energetic shifts of CT states or energy relaxation to the lowest CT band, to name just a few of them, which in turn has an impact on the  $V_{OC}$ .

### 3. Strategies to reduce energy losses

According to the different sources of energy losses in OPVs one can follow miscellaneous strategies to reduce them: (1) by reducing the CT strength  $\alpha_{CT}$ , (2) by reducing the driving force  $\Delta E_{CT}$ , and (3) by reducing non-radiative recombination.

#### 3.1. Reducing the CT strength

As predicted by the above described simulations, one approach consists in changing the absorption strength of the CT state. As explained in detail in the literature,  $\alpha_{CT}$  contains two contributions: one is the density of CT states per unit volume and the second is given by the electronic coupling strength between donor and acceptor [14]. **Figure 2(a)** schematically shows how both properties can be controlled, either by changing the morphology or by varying the relative molecular orientation. However, in a bulk heterojunction (BHJ) donor and

acceptor can exhibit a rich variety of phases, including neat phases of both of them on different length scales together with mixed phases of various compositions. Control over the BHJ morphology can be difficult as it requires also a precise determination of the morphology from the molecular to the mesoscopic scale. By contrast, a so-called planar heterojunction (PHJ) may still not have a perfectly flat D-A interface, but the contact area of both components is drastically reduced. Such an interface is well suited to study the effect of molecular orientation, provided that one is able to grow both materials in a reliable highly ordered, crystalline fashion on top of each other. However, recent work has shown that even in the case of prototypical “model systems” the interface can exhibit non-idealities, like intermixing or disorder, such that it is no longer an abrupt clean interface [25]. This is schematically shown in the right part of Figure 2(a) and should be kept in mind for the discussion below.

In both cases, BHJ and PHJ, the use of advanced x-ray scattering techniques such as grazing incidence small angle x-ray scattering (GISAXS) and grazing incidence wide angle x-ray scattering (GIWAXS) have proven to be very powerful to access the relevant structural information [26]. With GIWAXS the crystalline part is probed and crystal structure as well as crystal orientation with respect to the electrodes can be determined. With GISAXS the mesoscopic domain morphology can be comprehensively characterized. In addition, with polarized resonant soft X-ray scattering (P-SoXS) the orientation of molecules at interfaces can be determined also in case of non-planar interfaces and for non-crystalline interfaces [27]. Figure 2(b) exemplarily shows chemical structures of molecular materials that allow studying such effects (for further information we refer to [28-30]). In the first example (Figure 2(c)), we compare PHJ and BHJ solar cells consisting of DIP as donor and the fullerene C<sub>60</sub> as acceptor. Detailed x-ray scattering and optical studies have revealed that DIP grows crystalline with almost upright standing orientation of its long axis in both cases of PHJ and BHJ configuration – leading to exceptional excitonic transport properties – and that the main absorber is the fullerene (which also has the smaller gap of both  $E_g \approx 1.9$  eV) [28, 31]. While the PHJ has a smooth D-A interface, phase separation is observed in the BHJ; in both cases domain sizes depend on the details of the preparation conditions, particularly the temperature of the substrate during film growth. The current density-voltage ( $j$ - $V$ ) characteristics in Figure 2(c) show obvious differences between both configurations. While  $j_{SC}$  is higher in the BHJ,  $V_{OC}$  and  $FF$  are larger in the PHJ case. These distinctions are a consequence of the different D-A interfacial area in the two device architectures. Owing to a short exciton diffusion length of only 10-20 nm in C<sub>60</sub>, the BHJ generates more current due to a larger interface but also

gives rise to higher non-geminate recombination losses, reducing the  $FF$ . The difference in  $V_{OC}$  can be ascribed to the effect of  $\alpha_{CT}$ , which is of the order of  $10^{-3}$  in the BHJ with phase separation on 10-100 nm length scale, while it is about an order of magnitude lower in the PHJ [13]. Actually, in the BHJ part of the  $V_{OC}$  loss is compensated by the higher photocurrent, since  $V_{OC}$  depends logarithmically on  $j_{sc}$ . Thus, the difference under equal carrier densities is even slightly larger than apparent from Figure 2(c) at first glance.

In a similar manner, the density of interfacial CT states can be varied by dilution. Vandewal et al. have reduced the donor content in a matrix of  $C_{60}$  from 10% down to only 1% and observed a continuous increase in  $V_{OC}$  by up to 150 mV [32]. Because the CT energy, as detected by optical spectroscopy, did not change, the effect could unambiguously be ascribed to a reduction in  $\alpha_{CT}$ .

Another approach to modify  $\alpha_{CT}$  consists in changing the relative orientation of D and A molecules at the interface of a PHJ. In particular, the face-on orientation (lying molecules) vs. the edge-on orientation (standing molecules) – see Figure 2(a) – are expected to yield significantly different electronic couplings, because the conjugated  $\pi$ -system of the donor molecule is strongly exposed to the acceptor in the former case, while it is shielded in the latter case [33]. This effect is even more pronounced, if two rod-like molecules like 6T and DIP are used as donor and acceptor, respectively, because the orientation of molecules in the donor layer templates the alignment of molecules in the acceptor layer as well.

As shown in Figure 2(d), it is therefore possible to grow films with both lying and standing orientation on a non-heated substrate, while a heated substrate yields standing only orientation of both species. This results in a significant difference of  $V_{OC}$  of almost 0.2 eV at room temperature [29]. As verified by independent photoelectron and optical spectroscopy measurements the CT energetics are not affected by molecular orientation [29, 34]. Thus, the increase in  $V_{OC}$  has to be ascribed to the weaker electronic coupling in the edge-on configuration. Quantitative simulations of the temperature dependence of  $V_{OC}$  in both devices indeed confirm this notion and yield a difference in  $\alpha_{CT}$  of about three orders of magnitude [34].

Similar observations have been reported by other groups as well [35]. However, as demonstrated in these publications, care has to be taken to disentangle the effect of orientation dependent ionization energies and electron affinities on the one hand, and the actual differences in electronic couplings on the other hand [17]. Moreover, the importance of long-range electrostatic interactions should not be underestimated as well [36].



As already mentioned, D-A interfaces can be more complex than discussed above. There is evidence for intermixing in related systems like Pentacene/C<sub>60</sub> or Zn-Phthalocyanine/C<sub>60</sub> [25]. Furthermore, the coexistence of crystalline and amorphous phases of one or both partners at the D-A interface can have a significant influence on  $V_{OC}$  as well, as has been shown for Rubrene/C<sub>60</sub> and Squaraine/C<sub>60</sub> [24, 37].

### 3.2. Reducing the driving force

The most obvious approach for reducing energy losses is to minimize the driving force for CT formation. This can be achieved by varying the relative energy level positions at the D-A interface, e.g. by systematically changing the redox energies of a family of donor materials while keeping the acceptor fixed, or vice versa [38]. As already mentioned above, Li et al. have followed this approach and observed that the total energy loss cannot be reduced below 0.6 eV – otherwise the incident photon-to-current conversion efficiency (IPCE) starts to drop significantly [19].

At this point, we want to add that the energetics, i.e. the ionization energies and electron affinities as well as the CT state energy itself, can shift significantly by the presence of intermixing leading to the coexistence of multiple phases at the D-A boundary, which can cause changes in  $V_{OC}$  by several 100 mV as compared to an ideal, molecularly sharp interface. Recent examples are again Pentacene/C<sub>60</sub> and 6T/C<sub>60</sub> [22, 39].

A common way to quantify the charge transfer energy loss  $\Delta E_{CT}$  directly is to detect the position of the CT band relative to the optical gap. Several authors have shown that  $\Delta E_{CT}$  can approach zero for suitably chosen D-A pairs, which means that sensitive detection of the photocurrent as well as the EL spectra do no longer exhibit a distinct signature of CT states but only show absorption and emission across the fundamental gap of the absorber [34, 40]. However, only few of these cells still have high IPCE and PCE [41].

Another means of increasing the  $V_{OC}$  of OPVs is the implementation of interlayers. Instead of a single D-A heterojunction one or more additional layers are inserted between donor and acceptor so that the lowest unoccupied and the highest occupied molecular orbitals (LUMO / HOMO) of all materials form an energy cascade [42]. Thus, instead of a single-step charge transfer, which would be accompanied by a large energy loss, the CT process is split into several steps – so to speak – with much smaller overall loss. This concept is of general applicability and, in many cases, the interlayer can comprise even a derivative of the donor or acceptor compound, thereby, facilitating the morphological compatibility [42].

Figure 2(e) shows  $j$ - $V$  characteristics of a 6T/C<sub>60</sub> cell as an example, where the insertion of a thin DIP layer between both materials leads to a steady increase of  $V_{OC}$  with increasing DIP thickness. In this case, the effect of the DIP interlayer is twofold. It reduces the large energy loss for an electron transferred from 6T directly to C<sub>60</sub> ( $V_{OC} = 0.42$  eV) by providing an intermediate energy level on DIP. However, as the corresponding 6T/DIP and DIP/C<sub>60</sub> cells exhibit much higher  $V_{OC}$ 's (1.22 eV and 0.91 eV, respectively), the main effect probably comes from suppressed recombination between 6T and C<sub>60</sub> by the interlayer, similar to the application of wide-gap insulating interlayers as reported in literature [43].

An alternative mechanism to the formation of an energy cascade has recently been suggested in polymer-fullerene bulk hetero-junctions [44]. These authors have proposed that the presence of an intermixed interface with locally enhanced CT energy creates a driving force for charge separation without loss in  $V_{OC}$ .

Much stronger effects have been reported by Cnops et al. for a three-layer structure of 6T/subNc/subPc showing a  $V_{OC} = 0.96$  eV, where the subPc layer provides an additional contribution to the photocurrent by transferring excitons to subNc [45]. This structure has recently been improved further by introducing an additional DBP layer – a derivative of the above discussed DIP – between 6T and subNc, yielding a  $V_{OC} = 1.18$  eV [46]. The authors have shown that the CT state energy in this four-layer cascaded cell is equal to the smallest gap ( $E_{CT} = E_{subNc} = 1.73$  eV) and, thus, that the total energy loss is 0.55 eV only.

In another work, the Janssen group has correlated IPCE and energy losses of polymer:fullerene BHJ cells, where the excitation was either on the polymer or on the fullerene [47]. Surprisingly, they found that excitation of the fullerene is accompanied by a substantially larger energy loss (at least 0.85 eV), while the threshold for efficient cells after excitation of the donor polymer can be slightly less than 0.6 eV. Although the microscopic origin for this significant difference is not clear yet, other groups have reported further examples of remarkably small energy losses using non-fullerene acceptors [48].

### 3.3. Reducing the non-radiative recombination

The least attention, so far, has been paid to the third loss term in Equation (3), which is actually the most important one: the non-radiative recombination losses. As Vandewal and Tvingstedt et al. have pointed out, those can be as large as 0.35-0.40 eV in polymer:fullerene BHJ cells, where the radiative loss is 0.24 eV only [7, 14]. As discussed in the context of Equation (3), the magnitude of non-radiative losses is related to the overall very low quantum

efficiency of EL from CT states. However, the exact origin of the low  $\eta_{\text{EL}}$  remained elusive for a long time.

Only recently, Benduhn et al. [49] have suggested to apply “the energy gap law for radiationless transitions” reported by Englman and Jortner in 1970 [50] to CT emission. They observed that the empirical relation  $q \cdot V_{\text{OC}} = E_{\text{CT}} - 0.6 \text{ eV}$  is not strictly valid when data over a large range of CT energies are analyzed. Actually, the slope between  $V_{\text{OC}}$  and  $E_{\text{CT}}$  is slightly larger than 1, indicating that there is an energy dependence of the non-radiative loss term, as predicted by Englman and Jortner. In simple words, the non-radiative decay rate  $k_{\text{nr}}$  depends on the energy of the excited state, because the higher the latter is the more vibrational quanta  $\hbar\omega$  are needed for dissipation and, thus, the lower is  $k_{\text{nr}}$ :  $k_{\text{nr}} \propto \exp\left(-\frac{E_{\text{CT}}}{\hbar\omega}\right)$ . As demonstrated by Benduhn et al., the effect of non-radiative recombination losses in OPVs is quite dramatic, because  $\Delta E_{\text{rec}}^{\text{nr}}$  can be as large as 0.55 eV for an  $E_{\text{CT}}$  of 0.6 eV, while it is only about half as large for  $E_{\text{CT}} = 1.6 \text{ eV}$  [49].

This mechanistic suggestion is a big step forward. Though it does not directly solve the problem of non-radiative losses, it could provide the necessary insights to guide materials science to tune CT states toward higher radiative decay efficiency. However, the challenge is not to increase the second loss term in Equation (3) – the radiative one – too much at the same time [51].

### 3.4. Overview of selected small molecule OPV cells

At the end of this section, we would like to give a brief overview of the materials and the progress that has been made over recent years in our groups. **Figure 3** shows a compilation of data for energy losses in small molecule OPVs. All of these cells have comparable (optical) energy gaps between 1.9 and 2.1 eV (in all cells with C<sub>60</sub> or DBP as absorber the gap is 1.9 eV; with DIP as absorber it is 2.1 eV). The diagram shows that the energy loss is particularly large in the case of 6T/C<sub>60</sub>, because almost 1 eV of energy is lost in the primary charge transfer step. This can be drastically reduced by choosing D-A pairs with better energy level matching, especially for the non-fullerene acceptors on the right-hand side, where a 6T/DBP cell has a CT loss of only 0.13 eV.

The recombination losses of all material combinations are between 0.5 and 0.6 eV, which means roughly the same within the error bars, except for two cases. The high-temperature grown 6T/DIP cell has the highest  $V_{\text{OC}} = 1.35 \text{ eV}$  and a recombination loss below 0.5 eV, most likely due to the upright standing orientation of both molecular species leading to reduced electronic coupling [29]. Also remarkable is the case of DBP/ZCl with a Zn-

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chlorodipyrin as acceptor having a recombination loss below 0.4 eV [40b]. This acceptor molecule can exhibit an intramolecular symmetry-breaking CT in the excited state, which might further reduce recombination losses.

#### 4. Conclusion

Our understanding of energy losses in OPVs has made huge progress in recent years and different strategies for reducing them have been developed. It has been demonstrated that the driving force for the primary charge transfer step from a molecular exciton on the absorbing species toward the formation of an interfacial CT state between donor and acceptor can be basically reduced to zero. However, the overall energy loss from the optical gap to the open-circuit voltage still has a lower bound of about 0.6 eV. In particular, non-radiative recombination losses from CT states are still not very well understood, although they amount for the largest loss term. Thus, the way to reduce energy losses in OPVs below this limit is by no means obvious, but will require concerted efforts in materials design, device engineering together with improving experimental detection techniques as well as theoretical modelling.

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#### References

- [1] C. W. Tang, Two-layer organic photovoltaic cell, *Applied Physics Letters*, **1986**, *48*, 183.
- [2] National Renewable Energy Laboratory (NREL): Efficiency chart (Rev. 12-02-2016), [http://www.nrel.gov/pv/assets/images/efficiency\\_chart.jpg](http://www.nrel.gov/pv/assets/images/efficiency_chart.jpg), January 2017.
- [3] K. Leo, Organic photovoltaics, *Nature Reviews Materials*, **2016**, *1*, 16056.
- [4] ITRPV Working Group, International Technology Roadmap for Photovoltaic (ITRPV) Seventh Edition, 2016.
- [5] Perovskite Photovoltaics, *MRS Bulletin*, **2015**, *40*.
- [6] a) R. R. King, D. Bhusari, A. Boca, D. Larrabee, X.-Q. Liu, W. Hong, C. M. Fetzer, D. C. Law & N. H. Karam, Band gap-voltage offset and energy production in next-generation multijunction solar cells, *Progress in Photovoltaics: Research and Applications*, John Wiley & Sons, Ltd., **2011**, *19*, 797-812 b) M. A. Green, Radiative efficiency of state-of-the-art photovoltaic cells, *Progress in Photovoltaics: Research and Applications*, **2012**, *20*, 472-476.

Published in Advanced Energy Materials 7 (2017)1700237

- [7] K. Tvingstedt, O. Malinkiewicz, A. Baumann, C. Deibel, H. J. Snaith, V. Dyakonov & H. J. Bolink, Radiative efficiency of lead iodide based perovskite solar cells, *Scientific Reports*, **2014**, 4.
- [8] R. A. J. Janssen & J. Nelson, Factors Limiting Device Efficiency in Organic Photovoltaics, *Advanced Materials*, **2013**, 25, 1847-1858.
- [9] M. A. Ruderer, S. Guo, R. Meier, H.-Y. Chiang, V. Körstgens, J. Wiedersich, J. Perlich, S. V. Roth, P. Müller-Buschbaum, *Advanced Functional Materials*, **2011**, 21, 3382.
- [10] a) S. R. Forrest, The Limits to Organic Photovoltaic Cell Efficiency, *MRS Bulletin*, **2005**, 30, 28-32; b) M. Riede, T. Mueller, W. Tress, R. Schueppel, K. Leo, Small-molecule solar cells – status and perspectives, *Nanotechnology*, **2008**, 19, 424001; c) J.-L. Brédas, J. E. Norton, J. Cornil & V. Coropceanu, Molecular Understanding of Organic Solar Cells: The Challenges, *Accounts of Chemical Research*, **2009**, 42, 1691-1699; d) C. Deibel & V. Dyakonov, Polymer–fullerene bulk heterojunction solar cells, *Reports on Progress in Physics*, **2010**, 73, 096401; e) C. W. Schlenker & M. E. Thompson, The Molecular Nature of Photovoltage Losses in Organic Solar Cells, *Chemical Communications*, **2011**, 47, 3702-3716; f) K. Leo (Ed.), Elementary Processes in Organic Photovoltaics, *Advances in Polymer Science* 272, Springer **2017**.
- [11] W. Shockley & H. J. Queisser, Detailed balance limit of efficiency of p-n junction solar cells, *Journal of Applied Physics*, **1961**, 32, 510-519.
- [12] a) T. Kirchartz, J. Mattheis & U. Rau, Detailed balance theory of excitonic and bulk heterojunction solar cells, *Physical Review B*, **2008**, 78, 235320; b) N. C. Giebink, G. P. Wiederrecht, M. R. Wasielewski & S. R. Forrest, Thermodynamic efficiency limit of excitonic solar cells, *Physical Review B*, **2011**, 83, 195326; c) L. J. A. Koster, S. E. Shaheen & J. C. Hummelen, Pathways to a New Efficiency Regime for Organic Solar Cells, *Advanced Energy Materials*, **2012**, 2, 1246-1253.
- [13] M. Gruber, J. Wagner, K. Klein, U. Hörmann, A. Opitz, M. Stutzmann & W. Brütting, Thermodynamic Efficiency Limit of Molecular Donor-Acceptor Solar Cells and its Application to Diindenoperylene/C<sub>60</sub>-Based Planar Heterojunction Devices, *Advanced Energy Materials*, **2012**, 2, 1100-1108.
- [14] a) K. Vandewal, K. Tvingstedt, A. Gadisa, O. Inganäs & J. V. Manca, Relating the open-circuit voltage to interface molecular properties of donor:acceptor bulk heterojunction solar cells, *Physical Review B*, **2010**, 81, 125204 b) K. Vandewal, K. Tvingstedt, J. V. Manca & O. Inganäs, Charge-Transfer States and Upper Limit of the Open-Circuit Voltage in Polymer:Fullerene Organic Solar Cells, *Selected Topics in Quantum Electronics*, **2010**, 16, 1676-1684.
- [15] M. A. Green, Radiative efficiency of state-of-the-art photovoltaic cells, *Progress in Photovoltaics: Research and Applications*, **2012**, 20, 472-476.
- [16] a) A. Wilke, J. Endres, U. Hörmann, J. Niederhausen, R. Schlesinger, J. Frisch, P. Amsalem, J. Wagner, M. Gruber, A. Opitz, A. Vollmer, W. Brütting, A. Kahn & N. Koch, Correlation between interface energetics and open circuit voltage in organic photovoltaic cells, *Applied Physics Letters*, **2012**, 101, 233301; b) U. Hörmann, J. Kraus, M. Gruber, C. Schuhmair, T. Linderl, S. Grob, S. Kapfinger, K. Klein, M. Stutzman, H. J. Krenner & W. Brütting, Quantification of energy losses in organic solar cells from temperature-dependent device characteristics, *Physical Review B*, **2013**, 88, 235307
- [17] K. R. Graham, P. Erwin, D. Nordlund, K. Vandewal, R. Li, G. O. Ngongang Ndjawa, E. T. Hoke, A. Salleo, M. E. Thompson, M. D. McGehee & A. Amassian, Re-evaluating the Role of Sterics and Electronic Coupling in Determining the Open-Circuit Voltage of Organic Solar Cells, *Advanced Materials*, **2013**, 25, 6076-6082.

Published in *Advanced Energy Materials* 7 (2017)1700237

- [18] E. T. Hoke, K. Vandewal, J. A. Bartelt, W. R. Mateker, J. D. Douglas, R. Noriega, K. R. Graham, J. M. J. Fréchet, A. Salleo & M. D. McGehee, Recombination in Polymer:Fullerene Solar Cells with Open-Circuit Voltages Approaching and Exceeding 1.0 V, *Advanced Energy Materials*, **2013**, 3, 220-230
- [19] W. Li, K. H. Hendriks, A. Furlan, M. M. Wienk & R. A. J. Janssen, High Quantum Efficiencies in Polymer Solar Cells at Energy Losses below 0.6 eV, *Journal of the American Chemical Society*, **2015**, 137, 2231-2234.
- [20] T. Kirchartz, K. Taretto & U. Rau, Efficiency Limits of Organic Bulk Heterojunction Solar Cells, *The Journal of Physical Chemistry C*, 2009, 113, 17958-17966.
- [21] T. M. Burke, S. Sweetnam, K. Vandewal & M. D. McGehee, Beyond Langevin Recombination: How Equilibrium Between Free Carriers and Charge Transfer States Determines the Open-Circuit Voltage of Organic Solar Cells, *Advanced Energy Materials*, 2015, 5, 1500123.
- [22] K. R. Graham, G. O. N. Ndjawa, S. M. Conron, R. Munir, K. Vandewal, J. J. Chen, S. Sweetnam, M. E. Thompson, A. Salleo, M. D. McGehee & A. Amassian, The Roles of Structural Order and Intermolecular Interactions in Determining Ionization Energies and Charge-Transfer State Energies in Organic Semiconductors, *Advanced Energy Materials*, 2016, 6, 1601211.
- [23] X. Liu, K. Ding, A. Panda & S. R. Forrest, Charge Transfer States in Dilute Donor–Acceptor Blend Organic Heterojunctions, *ACS Nano*, 2016, 10, 7619-7626.
- [24] G. O. Ngongang Ndjawa, K. R. Graham, S. Mollinger, D. M. Wu, D. Hanifi, R. Prasanna, B. D. Rose, S. Dey, L. Yu, J.-L. Brédas, M. D. McGehee, A. Salleo & A. Amassian, Open-Circuit Voltage in Organic Solar Cells: The Impacts of Donor Semicrystallinity and Coexistence of Multiple Interfacial Charge-Transfer Bands, *Advanced Energy Materials*, 2017, 1601995.
- [25] a) Y.-T. Fu, C. Risko & J.-L. Brédas, Intermixing at the Pentacene-Fullerene Bilayer Interface: A Molecular Dynamics Study, *Advanced Materials*, WILEY-VCH Verlag, 2013, 25, 878-882 b) G. O. Ngongang Ndjawa, K. R. Graham, R. Li, S. M. Conron, P. Erwin, K. W. Chou, G. F. Burkhard, K. Zhao, E. T. Hoke, M. E. Thompson, M. D. McGehee & A. Amassian, Impact of Molecular Orientation and Spontaneous Interfacial Mixing on the Performance of Organic Solar Cells, *Chemistry of Materials*, 2015, 27, 5597-5604.
- [26] a) P. Müller-Buschbaum, Grazing incidence small-angle X-ray scattering: an advanced scattering technique for the investigation of nanostructured polymer films, *Analytical and Bioanalytical Chemistry*, **2003**, 376, 3-10 b) P. Müller-Buschbaum, The active layer morphology of organic solar cells probed with grazing incidence scattering techniques, *Advanced Materials*, **2014**, 26, 7692-7709 c) A. Hexemer & P. Müller-Buschbaum, Advanced grazing-incidence techniques for modern soft-matter materials analysis, *IUCrJ*, **2015**, 2, 106-125.
- [27] a) B. Collins, J. Cochran, H. Yan, E. Gann, C. Hub, R. Fink, C. Wang, T. Schuettfort, C. McNeill, M. Chabinyk & H. Ade, Polarized X-ray scattering reveals non-crystalline orientational ordering in organic films, *Nature materials*, **2012**, 11, 536-543 b) C. M. Palumbiny, J. Schlipf, A. Hexemer, C. Wang & P. Müller-Buschbaum, The Morphological Power of Soap: How Surfactants Lower the Sheet Resistance of PEDOT: PSS by Strong Impact on Inner Film Structure and Molecular Interface Orientation, *Advanced Electronic Materials*, **2016**.
- [28] a) J. Wagner, M. Gruber, A. Hinderhofer, A. Wilke, B. Bröker, J. Frisch, P. Amsalem, A. Vollmer, A. Opitz, N. Koch, F. Schreiber and W. Brütting, High fill factor and open circuit voltage in organic photovoltaic cells with diindenoperylene as donor material, *Advanced Functional Materials*, **2010**, 20, 4295; b) M. Gruber, M. Rawolle, J. Wagner, D. Magerl, U.

Published in Advanced Energy Materials 7 (2017)1700237

Hörmann, J. Perlich, S. V. Roth, A. Opitz, F. Schreiber, P. Müller-Buschbaum & W. Brütting, Correlating Structure and Morphology to Device Performance of Molecular Organic Donor–Acceptor Photovoltaic Cells Based on Diindenoperylene (DIP) and C<sub>60</sub>, *Advanced Energy Materials*, **2013**, 3, 1075-1083

[29] U. Hörmann, C. Lorch, A. Hinderhofer, A. Gerlach, M. Gruber, J. Kraus, B. Sykora, S. Grob, T. Linderl, A. Wilke, A. Opitz, R. Hansson, A. S. Anselmo, Y. Ozawa, Y. Nakayama, H. Ishii, N. Koch, E. Moons, F. Schreiber & W. Brütting, V<sub>oc</sub> from a Morphology Point of View: the Influence of Molecular Orientation on the Open Circuit Voltage of Organic Planar Heterojunction Solar Cells, *The Journal of Physical Chemistry C*, **2014**, 118, 26462-26470

[30] A. Steindamm, M. Brendel, A. K. Topczak & J. Pflaum, Thickness dependent effects of an intermediate molecular blocking layer on the optoelectronic characteristics of organic bilayer photovoltaic cells, *Applied Physics Letters*, **2012**, 101, 143302.

[31] a) A. K. Topczak, T. Roller, B. Engels, W. Brütting & J. Pflaum, Nonthermally activated exciton transport in crystalline organic semiconductor thin films, *Phys. Rev. B*, **2014**, 89, 201203; b) V. Settels, A. Schubert, M. Tafipolski, W. Liu, V. Stehr, A. K. Topczak, J. Pflaum, C. Deibel, R. F. Fink, V. Engel & B. Engels, Identification of Ultrafast Relaxation Processes As a Major Reason for Inefficient Exciton Diffusion in Perylene-Based Organic Semiconductors, *Journal of the American Chemical Society*, **2014**, 136, 9327-9337.

[32] K. Vandewal, J. Widmer, T. Heumüller, C. J. Brabec, M. D. McGehee, K. Leo, M. Riede & A. Salleo, Increased Open-Circuit Voltage of Organic Solar Cells by Reduced Donor-Acceptor Interface Area, *Advanced Materials*, **2014**, 26, 3839-3843.

[33] J.-L. Brédas, J. E. Norton, J. Cornil & V. Coropceanu, Molecular Understanding of Organic Solar Cells: The Challenges, *Accounts of Chemical Research*, **2009**, 42, 1691-1699.

[34] T. Linderl, U. Hörmann, S. Beratz, M. Gruber, S. Grob, A. Hofmann & W. Brütting, Temperature dependent competition between different recombination channels in organic heterojunction solar cells, *Journal of Optics*, **2016**, 18, 024007.

[35] B. P. Rand, D. Cheyng, K. Vasseur, N. C. Giebink, S. Mothy, Y. Yi, V. Coropceanu, D. Beljonne, J. Cornil, J.-L. Brédas & J. Genoe, The Impact of Molecular Orientation on the Photovoltaic Properties of a Phthalocyanine/Fullerene Heterojunction, *Advanced Functional Materials*, **2012**, 22, 2987-2995.

[36] C. Poelking, M. Tietze, C. Elschner, S. Olthof, D. Hertel, B. Baumeier, F. Würthner, K. Meerholz, K. Leo & D. Andrienko, Impact of mesoscale order on open-circuit voltage in organic solar cells, *Nature materials*, **2015**, 14, 434-439.

[37] J. D. Zimmerman, X. Xiao, C. K. Renshaw, S. Wang, V. V. Diev, M. E. Thompson & S. R. Forrest, Independent Control of Bulk and Interfacial Morphologies of Small Molecular Weight Organic Heterojunction Solar Cells, *Nano Letters*, **2012**, 12, 4366-4371.

[38] M. Brendel, S. Krause, A. Steindamm, A. K. Topczak, S. Sundarraj, P. Erk, S. Höhla, N. Fruehauf, N. Koch & J. Pflaum, The Effect of Gradual Fluorination on the Properties of F<sub>n</sub>ZnPc Thin Films and F<sub>n</sub>ZnPc/C<sub>60</sub> Bilayer Photovoltaic Cells, *Advanced Functional Materials*, **2015**, 25, 1565-1573.

[39] B. Yang, Y. Yi, C.-R. Zhang, S. G. Aziz, V. Coropceanu & J.-L. Brédas, Impact of Electron Delocalization on the Nature of the Charge-Transfer States in Model Pentacene/C<sub>60</sub> Interfaces: A Density Functional Theory Study, *The Journal of Physical Chemistry C*, **2014**, 118, 27648-27656.

[40] a) A. N. Bartynski, S. Grob, T. Linderl, M. Gruber, W. Brütting & M. E. Thompson, Organic Solar Cells with Open Circuit Voltage over 1.25 V Employing Tetraphenyldibenzoperiflanthene as the Acceptor, *The Journal of Physical Chemistry C*,

Published in *Advanced Energy Materials* 7 (2017)1700237

**2016**, 120, 19027-19034; b) A. N. Bartynski, M. Gruber, S. Das, S. Rangan, S. Mollinger, C. Trinh, S. E. Bradforth, K. Vandewal, A. Salleo, R. A. Bartynski, W. Brütting & M. E. Thompson, Symmetry-Breaking Charge Transfer in a Zinc Chlorodipyrin Acceptor for High Open Circuit Voltage Organic Photovoltaics, *Journal of the American Chemical Society*, **2015**, 137, 5397-5405.

[41] J. Liu, S. Chen, D. Qian, B. Gautam, G. Yang, J. Zhao, J. Bergqvist, F. Zhang, W. Ma, H. Ade, O. Inganäs, K. Gundogdu, F. Gao & H. Yan, Fast charge separation in a non-fullerene organic solar cell with a small driving force, *Nature Energy*, **2016**, 1, 16089.

[42] C. J. Mueller, M. Brendel, P. Ruckdeschel, J. Pflaum & M. Thelakkat, Diketopyrrolopyrroles with a Distinct Energy Level Cascade for Efficient Charge Carrier Generation in Organic Solar Cells, *Advanced Energy Materials*, **2015**, 5, 1500914.

[43] Y. Zhong, A. Tada, S. Izawa, K. Hashimoto & K. Tajima, Enhancement of  $V_{OC}$  without Loss of  $J_{SC}$  in Organic Solar Cells by Modification of Donor/Acceptor Interfaces, *Advanced Energy Materials*, **2014**, 4, 1301332.

[44] T. M. Burke & M. D. McGehee, How High Local Charge Carrier Mobility and an Energy Cascade in a Three-Phase Bulk Heterojunction Enable >90% Quantum Efficiency, *Advanced Materials*, **2014**, 26, 1923-1928.

[45] a) K. Cnops, B. P. Rand, D. Cheyns, & P. Heremans, Enhanced photocurrent and open-circuit voltage in a 3-layer cascade organic solar cell, *Applied Physics Letters*, **2012**, 101, 143301; b) K. Cnops, B. P. Rand, D. Cheyns, B. Verreet, M. A. Empl & P. Heremans, 8.4% efficient fullerene-free organic solar cells exploiting long-range exciton energy transfer, *Nature communications*, **2014**, 5, 3406.

[46] K. Vandewal, NGSEnano, Erlangen, (November, 2016); [http://www.bayern-innovativ.de/ngse2016\\_en](http://www.bayern-innovativ.de/ngse2016_en).

[47] K. H. Hendriks, A. S. G. Wijpkema, J. J. van Franeker, M. M. Wienk & R. A. J. Janssen, Dichotomous Role of Exciting the Donor or the Acceptor on Charge Generation in Organic Solar Cells, *Journal of the American Chemical Society*, **2016**, 138, 10026-10031.

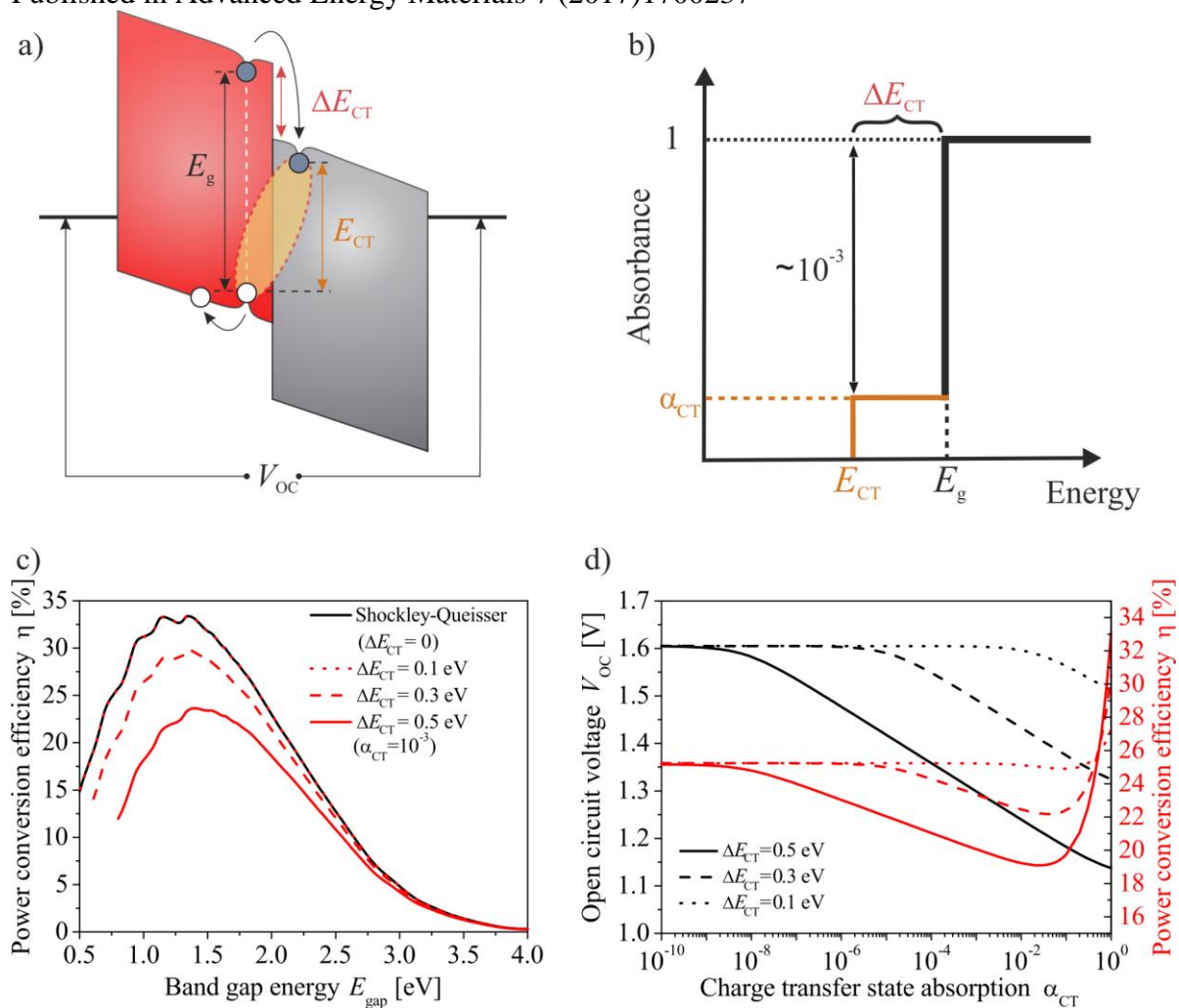
[48] a) Y. Fang, A. K. Pandey, A. M. Nardes, N. Kopidakis, P. L. Burn & P. Meredith, A narrow optical gap small molecule acceptor for organic solar cells. *Advanced Energy Materials*, **2013**, 3, 54-59; b) B. Verreet, K. Cnops, D. Cheyns, P. Heremans, A. Stesmans, G. Zango, C. G. Claessens, T. Torres & B. P. Rand, Decreased Recombination Through the Use of a Non-Fullerene Acceptor in a 6.4% Efficient Organic Planar Heterojunction Solar Cell. *Advanced Energy Materials*, **2014**, 4, 1301413; c) Z. Mao, W. Senevirathna, J.-Y. Liao, J. Gu, S. V. Kesava, C. Guo, E. D. Gomez, and G. Sauvé, Azadipyrromethene-Based Zn (II) Complexes as Nonplanar Conjugated Electron Acceptors for Organic Photovoltaics, *Advanced Materials*, **2014**, 26, 6290-6294.

[49] J. Benduhn, K. Tvingstedt, F. Piersimoni, S. Ullbrich, Y. Fan, M. Tropicano, K. A. McGarry, O. Zeika, M. K. Riede, C. J. Douglas, S. Barlow, S. R. Marder, D. Neher, D. Spoltore, K. Vandewal, Intrinsic non-radiative voltage losses in fullerene-based organic solar cells, *Nature Energy*, **2017**, 2, 17053.

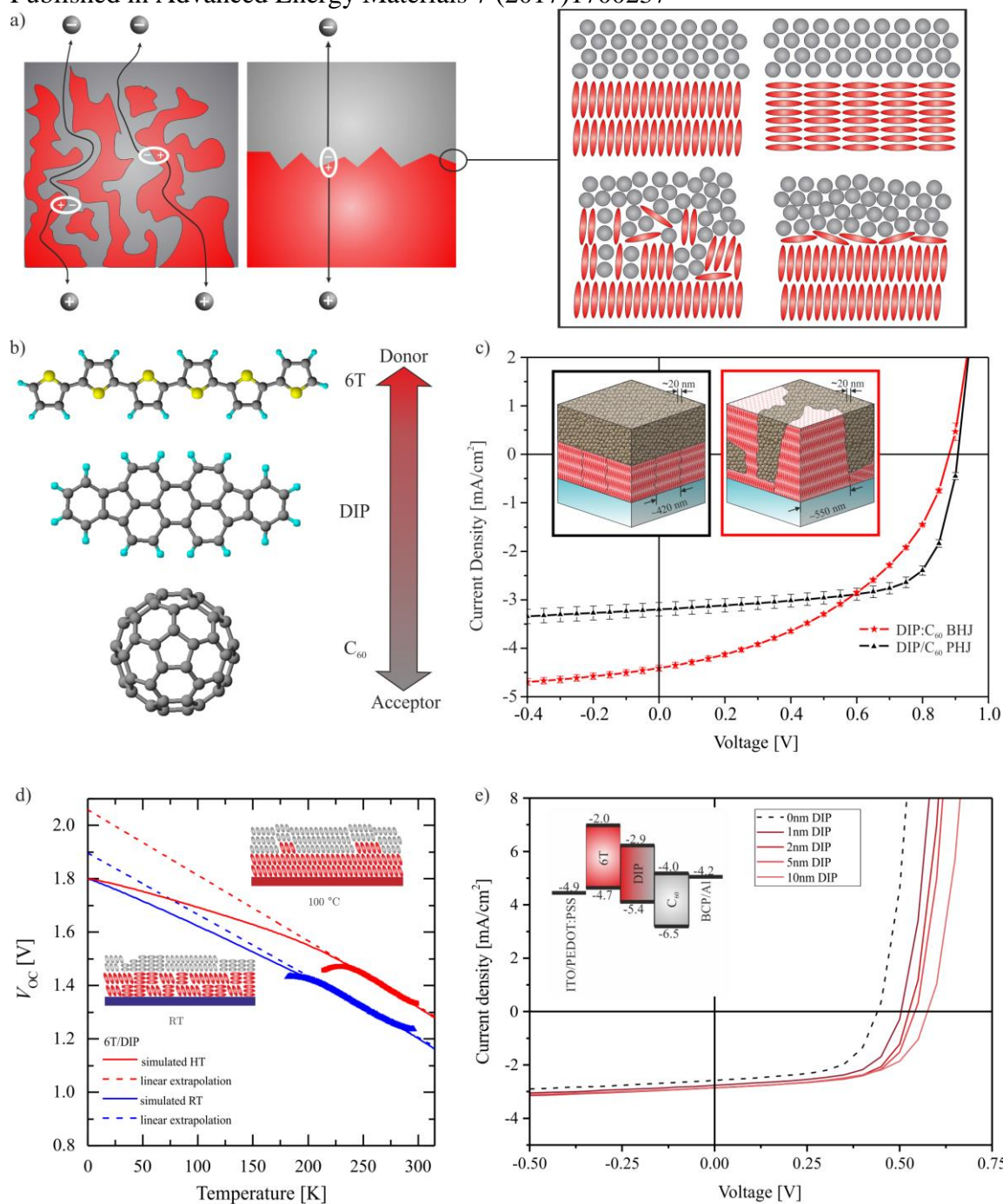
[50] R. Englman & J. Jortner, The energy gap law for radiationless transitions in large molecules, *Molecular Physics*, **1970**, 18, 145-164.

[51] K. Vandewal, Interfacial Charge Transfer States in Condensed Phase Systems, *Annual Review of Physical Chemistry*, **2016**, 67, 113-133.

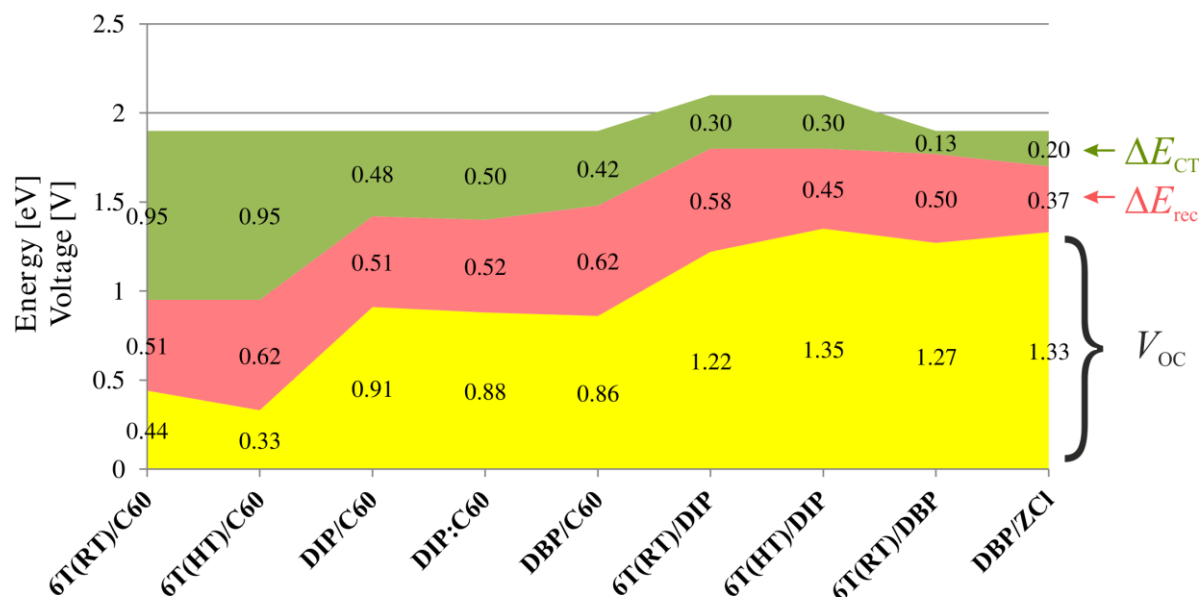




**Figure 1.** Working principle of an organic donor-acceptor (D-A) solar cell and predictions for their power conversion efficiency (PCE) as function of the energy and absorption strength of interfacial charge-transfer (CT) states. a) Schematic energy level diagram with photo-induced electron transfer from the donor at the left to the acceptor on the right. b) Simplified absorption spectrum with a subgap absorption step for CT states at the D-A interface. c) & d) Calculated PCE and  $V_{oc}$  following the modified Shockley-Queisser detailed balance approach with  $E_g = 1.9$  eV and, both,  $E_{CT}$  and  $\alpha_{CT}$  as variable parameters (for details see Ref. [13]). Reproduced with permission.<sup>[13]</sup> Copyright 2012, Wiley-VCH.



**Figure 2.** a) Schematic visualization of different interface morphologies in a bulk-heterojunction (BHJ) and a planar heterojunction (PHJ); for the latter, different molecular orientations can play a role as well, and the donor-acceptor interface can exhibit non-idealities such as intermixing or disorder. b) Chemical structures of some proto-typical small molecule semiconductors used for organic solar cells. c) Comparison of current-voltage characteristics and the corresponding morphology of DIP/C<sub>60</sub> BHJ (red) and PHJ (black) solar cells (for details see Ref. [28]). d) Temperature dependent  $V_{oc}$  of 6T/DIP solar cells with different relative orientation of the two compounds caused by different substrate temperature upon film growth (for details see Ref. [29, 34]). e) Current-voltage characteristics of cascaded solar cells with variable thickness of the DIP layer in between 6T and C<sub>60</sub>. Part (c) reproduced with permission.<sup>[28]</sup> Copyright 2013, Wiley-VCH.



**Figure 3.** Compilation of open-circuit voltages and the involved energy losses for selected small-molecule solar cells. The given numbers are taken from the following references: 6T/C<sub>60</sub> [16a, 29], DIP/C<sub>60</sub> [16b], DBP/C<sub>60</sub> [40a], 6T/DIP [29], 6T/DBP [40a], DBP/ZCl [40b]. RT and HT denote film deposition with the substrate at room temperature or at 100°C, respectively. All cells except for DIP:C<sub>60</sub>, which was a BHJ, were fabricated in PHJ architecture.

**TOC entry:**

**The energy loss between the optical gap and the open-circuit-voltage** is one of the primary reasons why the efficiency of organic photovoltaic cells lags behind their inorganic counterparts. This Research News highlights the scientific background and presents strategies to improve on this issue.

**Keyword: Organic Solar Cells**

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**Energy Losses in Small-Molecule Organic Photovoltaics**

