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The voltage loss in organic solar cells

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The power conversion efficiency (PCE) for donor–acceptor bulk-heterojunction organic solar cells (OSCs) has reached ~20%[1–3], approaching that for inorganic solar cells, due to the development of key photoactive materials[4–14]. The short-circuit current density (J_{sc}) and the fill factor (FF) for state-of-the-art OSCs are already close to the thermodynamic upper limit predicted by Shockley-Queisser theory[15], but the open-circuit voltage (V_{oc}) is low, limiting the overall performance of OSCs.

Low V_{oc} can be ascribed to the high radiative (V_r) and non-radiative (V_{nr}) voltage losses associated with the decay of photogenerated charge carriers[16]. Thus, understanding the mechanism of charge carrier decay dynamics in OSCs is the focus for device physicists. In 2009, Vandewal *et al.* analyzed the energetics of excited states in polymer-fullerene solar cells and revealed that the decay of charge carriers in OSCs occurred *via* the charge transfer (CT) states formed at the polymer-fullerene interface[17]. Therefore, the high voltage loss was associated with the undesired electronic properties of CT state. Later, Vandewal *et al.* demonstrated that the key parameters determining the voltage loss included the energy of CT state (E_{ct}), the reorganization energy (λ) of organic photovoltaic materials, and the absorption oscillator strength (f_{osc}) of CT state[18].

Owing to the existence of CT states with energy lower than the singlet (S_1) state of the pristine photovoltaic materials, the absorption tail of OSCs extends into the long wavelength region. This leads to a very high saturation current[19], yielding high V_r. Reducing the energy difference between the CT state and the S_1 state (ΔE_{ct}) is an effective approach to reduce V_r[19]. However, the reduced ΔE_{ct} often led to reduced exciton dissociation rate and limited device quantum efficiency[20]. Reducing the density of CT state (N_{ctc}) can also effectively reduce V_r[21]. The reduced N_{ctc} resulted in deteriorated transport properties of charge carriers, thus limiting FF. High V_r was believed to be an intrinsic problem for OSCs[22].

In non-fullerene solar cells, high quantum efficiency could be obtained by using donor–acceptor blends with very low ΔE_{ct} or low N_{ctc}[23]. Therefore, negligible V_r could be realized, and the major limit for V_{oc} is V_{nr}, which is associated with low external quantum efficiency of electroluminescence

(EQE$_{EL}$) for CT state[24], since

$$V_{nr} = \frac{kT}{q}\ln\left(\frac{1}{EQE_{EL}}\right),$$

where k is Boltzmann constant, q is elementary charge, and T is temperature. EQE$_{EL}$ is determined by following formula[25]:

$$EQE_{EL} = \frac{k_r}{k_r + k_{nr}},$$

where k_r and k_{nr} are the radiative and non-radiative decay rate constant, respectively. Thus, very high k_{nr} for CT state in organic blends leads to low EQE$_{EL}$. Low EQE$_{EL}$ (<1 × 10^{-5}) for organic solar cells yields high V_{nr} (>0.3 V)[26]. Accordingly, more efforts have been spent on the manipulation of the decay dynamics of CT state in recent years to reduce k_{nr} and increase EQE$_{EL}$. In 2017, Bunduhn *et al.* discovered that high k_{nr} of OSCs originated from strong vibrational coupling between CT state and the ground state[27]. The strong coupling resulted from high-frequency carbon vibration of organic molecules. Later, Ullbrich *et al.* reported that increasing E_{ct} could reduce vibrational coupling and reduce k_{nr}[28]. V_{nr} was very low in OSCs with high E_{ct}. However, the use of high-bandgap material for high E_{ct} led to reduced spectral coverage of the solar cell, and thus reducing J_{sc} and limiting overall device performance. Increasing the spacing between donor and acceptor molecules could also reduce k_{nr} and reduce V_{nr}, thus improving overall device performance[29]. Furthermore, Azzouzi *et al.* extended the model describing non-radiative decay rate of CT state[30], and demonstrated that reducing λ and f_{osc}, or increasing static dipole moment of CT state, could reduce k_{nr}.

Qian *et al.* indicated that increasing the degree of hybridization between CT state and S_1 state could effectively increase EQE$_{EL}$[31]. The increase in EQE$_{EL}$ was ascribed to the intensity-borrowing mechanism of the excited states. Later, Eisner *et al.* built a model to describe the impact of hybridization on the dynamic process of excited states[32]. They found that V_{nr} could be reduced, while increasing V_r. It is still unclear whether the hybridization could improve overall device performance.

Based on the improved understanding on V_{oc} loss mechanism, many strategies, such as ternary strategy[33], mixed-solvent strategy[23], and thin-film deposition strategy[34], as well as material design strategies (e.g. side-chain engineering[35], double-cable structure[36]) have been developed to reduce voltage loss. Now the lowest voltage loss is below 0.4 V[37].

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OSC performance will be further improved[38, 39], thus paving the road to real commercialization.

Acknowledgements

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