Electronic Supplementary Information

Acceptor-donor-acceptor type molecules for high performance organic photovoltaics – chemistry and mechanism

Xiangjian Wan,\textsuperscript{a,c} Chenxi Li,\textsuperscript{a} Mingtao Zhang,\textsuperscript{a} Yongsheng Chen \textsuperscript{*a,b,c}

\textsuperscript{a} The Centre of Nanoscale Science and Technology and Key Laboratory of Functional Polymer Materials, Institute of Polymer Chemistry, College of Chemistry, Nankai University, Tianjin 300071, China
\textsuperscript{b} State Key Laboratory of Elemento-Organic Chemistry, Nankai University, Tianjin, 300071, China
\textsuperscript{c} Renewable Energy Conversion and Storage Center (RECAST), Nankai University, Tianjin 300071, China

1. HOMO/LUMO calculation and analysis for some A-D-A molecules
2. A semi-empirical model analysis for PCE prediction

2.1 For the semi-empirical analysis based on a single cell, the fundamental assumptions are made as follows:

1) An internal quantum efficiency (IQE) of 100% is considered for the whole absorption wavelengths.\(^1\)

2) EQE is assumed to be same in the whole absorption range with a given value of 80% and FF is assumed to be 0.8.

3) In the discussion as follows, the optical gap of the subcell \(E_g\) (\(= 1240/\lambda_{onset}\)) is defined as the narrower optical gaps of the donor-acceptor couples. Note, for the
fullerene based devices, the absorption onset is considered to be that of the donor materials. For the fullerene-free based devices, it referred to be that of material, either donor or acceptor, whichever has a narrower bandgap.\textsuperscript{2}

Based on above assumptions, the three photovoltaic parameters $V_{oc}$, $J_{sc}$ and $FF$ of a single cell is obtained as follows:

1) For a single cell with absorption onset $\lambda$, the $J_{sc}$ of the cell could be obtained from equation 1 (Eq. 1).

\[
J_{sc} = \int_{\lambda}^{\infty} \frac{q \lambda}{h c} E(\lambda) \cdot EQE(\lambda) \cdot d \lambda
\]

(1)

where $E(\lambda)$ is the spectral irradiance in AM 1.5G, $\lambda$ is the absorption onset of the cell, $h$ is Planck's constant, $c$ is the speed of light and $q$ is the elementary charge.

2) The $V_{oc}$ of the cell is determined by the following Eq. 2.

\[
V_{oc} = \frac{1}{q} (E_{g} - E_{loss}) = \frac{1}{q} (\frac{1240}{\lambda} - E_{loss})
\]

(2)

The $E_{loss}$ are assumed to be 0.4-0.8 eV according to overall reported values.\textsuperscript{3}

So for the single cell, the PCE can be calculated from the Eq. 3 under AM 1.5G light illumination.

\[
PCE(%) = V_{oc} \cdot J_{sc} \cdot FF / P_{in}
\]

\[
= \frac{1}{q} (\frac{1240}{\lambda} - E_{loss}) \int_{\lambda}^{\infty} \frac{q \lambda}{h c} E(\lambda) \cdot EQE(\lambda) \cdot d \lambda \cdot FF / P_{in}
\]

(3)

2.2 For the semi-experimtal analysis based on a 2-terminal monolithic tandem cell with two subcells connected in series, the detailed description has been reported in literature.\textsuperscript{4} The Figure 7b in the ms is obtained under the given EQE of 80% and FF%. 
References:


