Solar cell efficiency as a function of blocking layer thicknesses and exciton fluorescence quantum yield

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Introduction

Contrary to their non-radiative counterpart, fluorescence losses strongly depend on the environment. By properly tuning the thicknesses of the buffer layers between the active regions of the cell and the electrodes, the exciton lifetime and, hence, the exciton diffusion length can be increased. Besides this effect, interferences within the cell control the efficiency of sunlight injection into the active layers. An optimal cell design must rely on the consideration of these two aspects [3].

The importance of the fluorescence losses depends on the fluorescent quantum yield, $q$, which is the fraction of the exciton decay that is intrinsically due to fluorescence:

$$ q = \frac{\Gamma_{\text{bulk}}}{\Gamma_{\text{bulk}}}$$

where $\Gamma_{\text{bulk}}$ and $\Gamma_{\text{bulk}}$ are the rate of radiative and non-radiative decay, respectively, and the ‘bulk’ subscript indicate that it is the bulk value. The bulk value of the radiative loss is an intrinsic quantity, which is obtained in the absence of boundary effects. In a confined environment such as in an organic cell, the actual radiative losses $\Gamma(z)$ generally differ from $\Gamma_{\text{bulk}}$ and depend on the position, $z$, of the exciton [2].

Generalized Shockley-Queisser theory

The I-V curve is given in term of the External Quantum Efficiency, EQE, by [1, 3]

$$ I(V) = \int_{0}^{\infty} \text{EQE}(\lambda, V) \exp \left( \frac{\hbar \lambda (\lambda - \lambda_0)}{kT} \right) d\lambda $$

where $\lambda$ is the wavelength, $\Omega$ is the solid angle of the sun, $\sigma_{\text{AM1.5}}$ is the AM1.5 solar spectrum and $T$ the cell temperature. The EQE can be calculated from the exciton diffusion equation

$$ \frac{\partial \rho}{\partial t} = - \Gamma(z, q) \rho + \frac{\partial}{\partial \lambda} \left( \Gamma(z, q) \frac{\partial \rho}{\partial \lambda} \right) $$

where $\rho$ is the exciton density, $D$ their diffusion coefficient and $q$ is the generation rate per photon and per unit length. In our computation of $\Gamma(z, q)$, we assumed that radiative excitons emit at 900nm, see [2] for more details.

With proper boundary conditions ($\partial \rho|_{z=0} = 0, \partial \rho|_{z=b} = 0$ and $\rho|_{z=b} = 1$), we determine the exciton density and hence the diffusive current at the donor/Acceptor/EBL interface which yields to the EQE as

$$ \text{EQE}(\lambda, V) = \int_{0}^{\infty} \frac{1}{\sigma_{\text{AM1.5}}} \left( \frac{\partial \rho}{\partial \lambda} \right)_{\lambda=\lambda_0} d\lambda $$

Once the curve I-V is determined, it is easy to compute the cell efficiency.

Numerical results 1 : high-efficiency cell

We consider the following cell: Ag|HBL(h)/Acceptor(Donor)/EBL|ITO/glass

with a favourable set of refractive indexes for increasing the exciton effective diffusion length through the management of the radiative losses. This set, together with layer thicknesses, is given in the accompanying table. Imaginary part of refractive index in acceptor and donor layer non-zero only for $\lambda \leq 300[\mu \text{m}, 700[\mu \text{m}].$

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness (nm)</th>
<th>Refract. Index</th>
<th>Diff. length</th>
</tr>
</thead>
<tbody>
<tr>
<td>Glass</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ITO</td>
<td>150</td>
<td>1.76±0.001</td>
<td></td>
</tr>
<tr>
<td>EBL</td>
<td>h</td>
<td>1.7</td>
<td></td>
</tr>
<tr>
<td>Donor</td>
<td>15</td>
<td>2.8±0.015</td>
<td>10</td>
</tr>
<tr>
<td>Acceptor</td>
<td>15</td>
<td>2.8±0.015</td>
<td>10</td>
</tr>
<tr>
<td>HBL</td>
<td>h</td>
<td>1.7</td>
<td></td>
</tr>
<tr>
<td>Ag</td>
<td>$\infty$</td>
<td>0.03±0.198</td>
<td></td>
</tr>
</tbody>
</table>

FIG 1. Power conversion efficiency $q$ as a function of blocking layer thicknesses, $h_1$ and $h_2$, for $q = 0, 0.05, 0.5, 1$ in both Acceptor and Donor layers.

FIG 2. Normalised exciton decay rate as a function of the distance from the back electrode for $(h_1, h_2) = (45[\mu \text{m}, 21[\mu \text{m}].$

Numerical results 2 : low efficiency cell

We now consider the following cell: Ag|BCP(h)/C60(31.5[\mu \text{m}])/DBP∗(10.5[\mu \text{m}])/MoO3(h)/ITO(250[\mu \text{m}])/glass, for which we use experimentally measured refractive indexes. C60∗ and DBP designate materials with identical complex refractive indexes to those of C60 and DBP, but where $q = 1$ is a free parameter. The diffusion length is 21[\mu \text{m}] in C60 and 7[\mu \text{m}] in DBP.

FIG 4. Power conversion efficiency $q$ as a function of $h_1$ and $h_2$ for $q = 0, 0.05, 0.5, 1$ in both Acceptor and Donor layers.

FIG 5. Normalised exciton decay rate in the active layers for different value of $q$ for $(h_1, h_2) = (25[\mu \text{m}, 21[\mu \text{m}].$

FIG 6. Power conversion efficiency $q$ as a function of radiative quantum efficiency $\eta$. Blue curve: $(h_1, h_2) = (25[\mu \text{m}, 21[\mu \text{m}].$ Red curve: $(h_1, h_2)$ set to optimal value for each $q$.

Conclusion

The main conclusion of this communication is that the cell architecture should be designed with proper account of $q$:

- In both Fig 1 and 4, there is a qualitative change as soon as $q > 0$. This is due to the quantum effects experienced by radiative excitons in the vicinity of a dissipative medium. This shows that to model the organic cell with $q = 0$ is an inaccurate modelling assumption.

- By properly managing fluorescence losses, one can significantly improve the cell performance. In our first example, the efficiency increase from 11.3% to 12.7%.

- Not to take into account the strong dependence of fluorescence on the environment may lead to a sub-optimal cell design and a degradation of cell performance. In our second example, the optimal configuration vary substantially with $q$.

For further improvements:

- Large-$\eta$ photofluorescent molecules with preferential dipole orientation seem to be a good candidate for further improvement but it is not sufficient in itself.

- A general rule to improve the efficiency is that the (real part of) refractive index contrast between the photofluorescent layers and the buffer layers should be large.

- With a ratio of 2.8, the efficiency increase from 11.3% to 12.7% in the best configuration for $q = 0$ and $q = 1$ respectively. But if the ratio is 2.8-1.45, the increasing go from 11.3% to 14.5%.

Remarks

- For the simplicity of this poster we neglect the angular dependence of processes, nevertheless, it is not the case in our calculation.

- We have considered some $q = 0$ in both acceptor and donor materials.

- We choose to maximise the cell efficiency by varying only the buffer thicknesses because they are easily tunable fabrication parameters.

- As we vary $q$, we keep the bulk diffusion length unchanged. So increasing $q$ don’t mean decreasing $\Gamma_{\text{diff}}$ or $\Gamma_{\text{bulk}}$ so as to compare active regions that would otherwise be equivalent.

- Molecules with large $\eta$ molecules with preferential dipole orientation and large buffer layers are already present in OLED.

References

