Ascertaining the Limitations of Low Mobility on Organic Solar Cell Performance

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INTRODUCTION

In the past decade, organic photovoltaics have emerged as an intensely studied alternative energy technology. The OPV platform presents several attractive qualities, yet, the high disorder and relative low mobility of the materials comprising OPV systems remains a bottleneck to further progress. We report in this abstract a modeling methodology that quantifies the efficiency losses engendered by the low mobility of these systems. We also report a methodology that explicitly treats the charge transfer (CT) state that has been shown to influence device performance. We compare two commonly studied OPV architectures, the bilayer (BL) and blended bulk-heterojunction (BHJ), and separately investigate the sensitivity of each architecture to mobility.

METHODOLOGY

Exciton (X), Charge transfer state (I), electron (n) and hole (p) dynamics are treated within the traditional continuity equation framework (Eqs. 2-5), where the electric field (F) is treated self-consistently via Poisson's equation (Eq. 1):

$$\varepsilon_0 \varepsilon_r \frac{\partial F}{\partial x} = q(p(x) - n(x)) \; ; \quad F(x) = -\frac{\partial \phi}{\partial x} \tag{1}$$

$$\frac{\partial X}{\partial t} = G(x) - k_{cap}(x)X(x) + \frac{\mu_X k_B T_0}{q}\frac{\partial^2 X}{\partial x^2} - k_{R,X}X(x) \tag{2}$$

$$\frac{\partial I}{\partial t} = k_{cap}(x)X(x) - D(F,I,x) - k_{R,I}I(x) \tag{3}$$

$$\frac{\partial n}{\partial t} = D(F,I,x) - R(n,p) + \frac{\mu_n}{q}\frac{\partial}{\partial x}\left[qnF + k_B T_0 \frac{\partial n}{\partial x}\right] \tag{4}$$

$$\frac{\partial p}{\partial t} = D(F,I,x) - R(n,p) - \frac{\mu_p}{q}\frac{\partial}{\partial x}\left[qpF - k_B T_0 \frac{\partial p}{\partial x}\right] \tag{5}$$

The quantities G, D, and R are the exciton photogeneration rate, the exciton dissociation rate, and the carrier recombination rate, resp. G is determined by the experimental photon flux, D is modeled using Braun's adaptation of Onsager's theory of geminate dissociation, and R is the traditional Langevin bimolecular recombination rate. Explicit incorporation of the CT state dynamics is unique to this study.

DEVICE SIMULATION

A one-dimensional model is used, with a simulated device thickness (d) of 100 nm. Four series of simulations are conducted: two series on the BL architecture and two series on the BHJ architecture. The BL architecture is treated by restricting D to take a non-zero value only at x=d/2, whereas the BHJ is simulated by permitting dissociation throughout the domain of x. The effect of mobility on device performance is investigated by varying the electron (μ_n) and hole mobility (μ_p) from 10^{-9} to 10^{-4} $m^2 \cdot V^{-1} \cdot s^{-1}$ while holding them equal. The relative performance enhancements in the BL and BHJ architectures are reported. The effect of a mobility mismatch ($\mu_n \neq \mu_p$) is also investigated by taking $\mu_n = 10^{-9}$ $m^2 \cdot V^{-1} \cdot s^{-1}$ while keeping $\mu_p = 10^{-4}$ $m^2 \cdot V^{-1} \cdot s^{-1}$

DISCUSSION

The simulations indicate that efficiency enhancements can be achieved by moving to higher mobility materials. Interestingly, we observe a maximal mobility above which dark current and recombination via the Langevin term results in a net reduction of performance. Finally, optimal performance is observed when the mobility of both components match, indicating that increasing the mobility of only one component can, in fact, hurt performance.

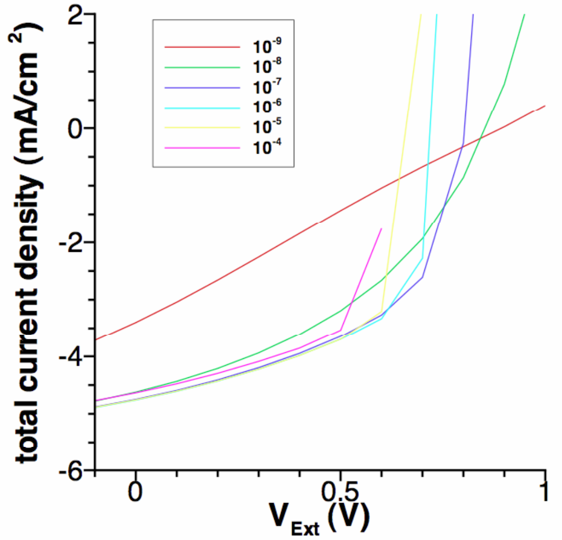

Fig. 1. Bilayer system simulations where $\mu_n=\mu_p$. The mobility is varied from $\mu=10^{-9}$-10^{-4} $m^2\bullet V^{-1}\bullet s^{-1}$, the device thickness, d, is 100 nm, and the incident photon flux (Γ_0) is $1x10^{21}$ $photons\bullet m^{-2}\bullet s^{-1}$. Optimal performance (as measured by the maximal product of $-V_{ext}\bullet J$, where J is the current density) is obtained for the $\mu=10^{-7}$ $m^2\bullet V^{-1}\bullet s^{-1}$ simulation. Increases in μ above 10^{-7} $m^2\bullet V^{-1}\bullet s^{-1}$, leads to reduced open circuit voltage (x intercept) due to dark current enhancement.

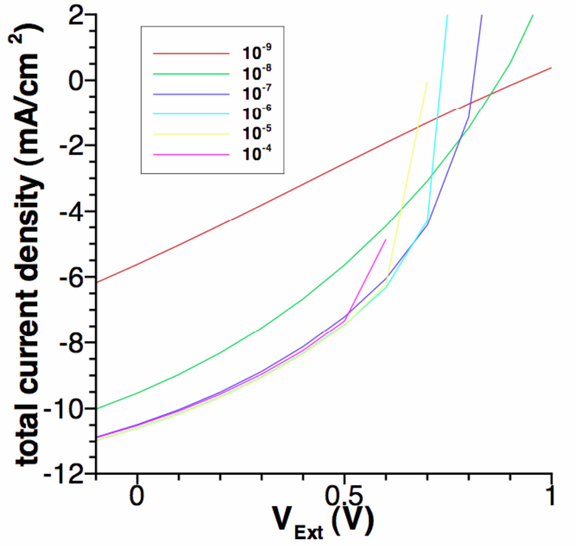

Fig. 2. Bulk Heterojunction system simulations where $\mu_n=\mu_p$. The mobility is varied from $\mu=10^{-9}$-10^{-4} $m^2\bullet V^{-1}\bullet s^{-1}$, the device thickness (d) is 100 nm, and the incident photon flux (Γ_0) is $1x10^{21}$ $photons\bullet m^{-2}\bullet s^{-1}$. The optimal mobility is found to be $\mu=10^{-7}$. The BHJ shows a pronounced photocurrent enhancement at higher mobilities, accenting the important of langevin recombination in this architecture.

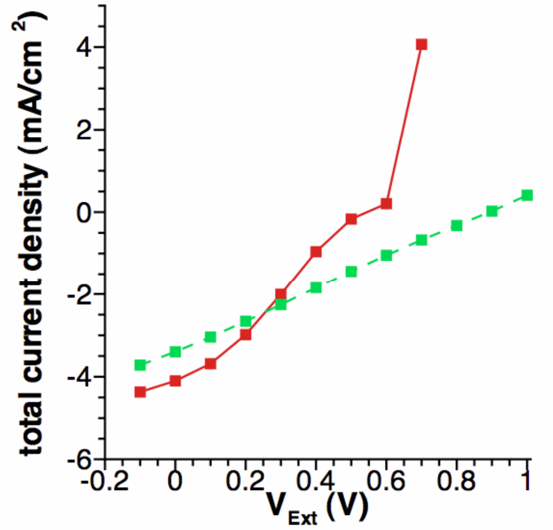

Fig. 3. Bilayer system simulations for $\mu_n\neq\mu_p$. Solid (Red): $\mu_n=10^{-9}$ $m^2\bullet V^{-1}\bullet s^{-1}$ and $\mu_p=10^{-4}$ $m^2\bullet V^{-1}\bullet s^{-1}$; Dashed (Green): $\mu_n=\mu_p=10^{-9}$ $m^2\bullet V^{-1}\bullet s^{-1}$. Mismatched mobility results in an improved short-cicuit current (y-intercept) but leads to a compensating reduction in open circuit voltage (x-intercept).

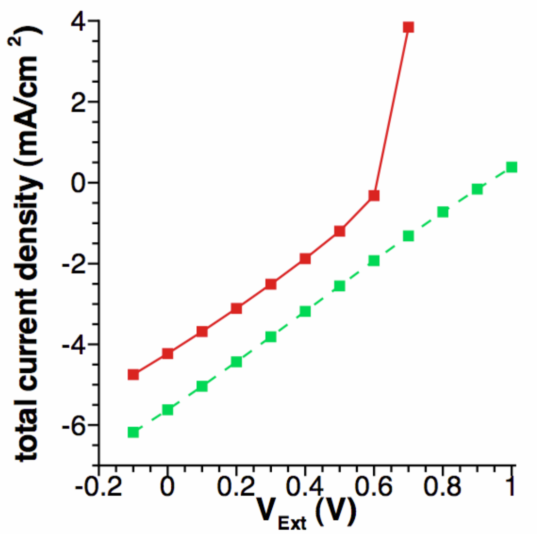

Fig. 4. Bulk heterojunction system simulations for $\mu_n\neq\mu_p$. Solid (Red): $\mu_n=10^{-9}$ $m^2\bullet V^{-1}\bullet s^{-1}$ and $\mu_p=10^{-4}$ $m^2\bullet V^{-1}\bullet s^{-1}$; Dashed (Green): $\mu_n=\mu_p=10^{-9}$ $m^2\bullet V^{-1}\bullet s^{-1}$. Mismatched mobility results both open-circuit voltage (x-intercept) and photocurrent losses, unlike the bilayer system that showed some current enhancement.