Research Update Solar Cell Simulation Code

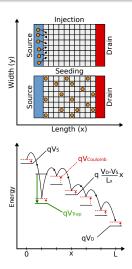
 $\underset{\tiny \mathsf{agg7@pitt.edu}}{\mathsf{Adam}} \; \mathsf{Gagorik}$

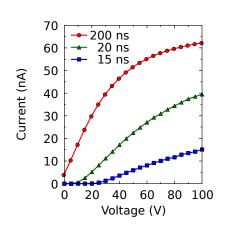
Department of Chemistry University of Pittsburgh

February 14, 2012

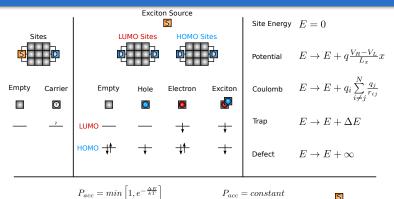
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Langmuir (OFET Model)





Langmuir (OFET Model and OPV Model)













 $P_{acc} = constant$

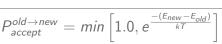
 $P_{acc} = 0$

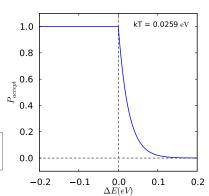
 $P_{acc} = constant$

Monte Carlo

$$P_{propose}^{old \rightarrow new} \times P_{accept}^{old \rightarrow new} \times P_{old} = P_{propose}^{new \rightarrow old} \times P_{accept}^{new \rightarrow old} \times P_{new}$$

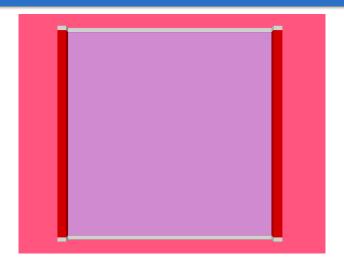
$$P_{propose}^{old o new} = P_{propose}^{new o old}$$
 $P_{old} \propto e^{rac{-E_{old}}{kT}}$
 $P_{new} \propto e^{rac{-E_{new}}{kT}}$
 $P_{new} = min \left[1.0, e^{rac{-(E_{new} - E_{old})}{kT}}
ight]$







Movie



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AM1.5 (Estimating Injection Rate)

Area
$$[m^2] \frac{\lambda}{hc} \left[\frac{\text{photon}}{J} \right] \int_0^{\infty} Irradiance \left[\frac{J}{s*m^2*nm} \right] \times e^{-\frac{(x-\bar{x})^2}{2\sigma}} d\lambda [nm]$$

2.5

2.0

253.633729212 W/m**2

0.5

0.0

0.5

0.0

1000 1500 2000 2500 3000 3500 4000 Wavelength (nm)

AM1.5 (Estimating Injection Rate)

Area
$$\begin{bmatrix} m^2 \end{bmatrix} \frac{\lambda}{hc} \begin{bmatrix} \frac{photon}{J} \end{bmatrix} \int_0^{\infty} Irradiance \begin{bmatrix} \frac{J}{s*m^2*nm} \end{bmatrix} \times e^{-\frac{(x-\bar{x})^2}{2\sigma}} d\lambda [nm]$$

1.00e-03

ETR

Global Tilt

Direct Circumsolar

4.00e-04

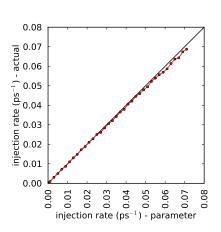
2.00e-04

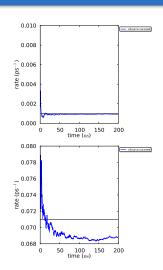
2.00e-04

Area (nm^2)

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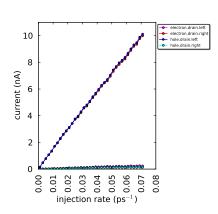
Exciton Injection Rate

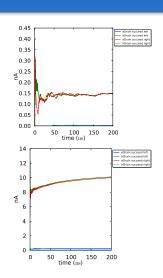






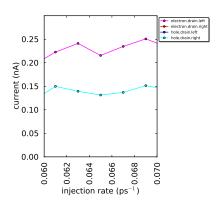
Current at the Electrodes

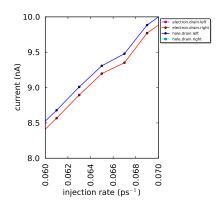




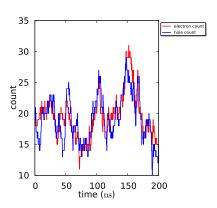


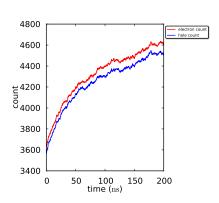
Current at the Electrodes Zoomed In





Charge Imbalance?





Thoughts on Imbalance

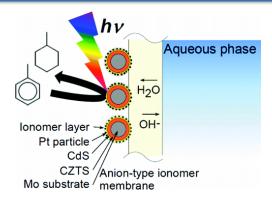
$$if (Electron) \&\& HOMO(site) == Hole$$

 $E_{Coulomb} += contant;$



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Questions?



P. Wang et al. "Photoelectrochemical Conversion of Toluene to Methylcyclohexane as an Organic Hydride by Cu2ZnSnS4-Based Photoelectrode Assemblies". In: *Journal of the American Chemical Society* (2012). DOI: 10.1021/ja209869k