Research Update

Solar Cell Simulation Code

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February 14, 2012

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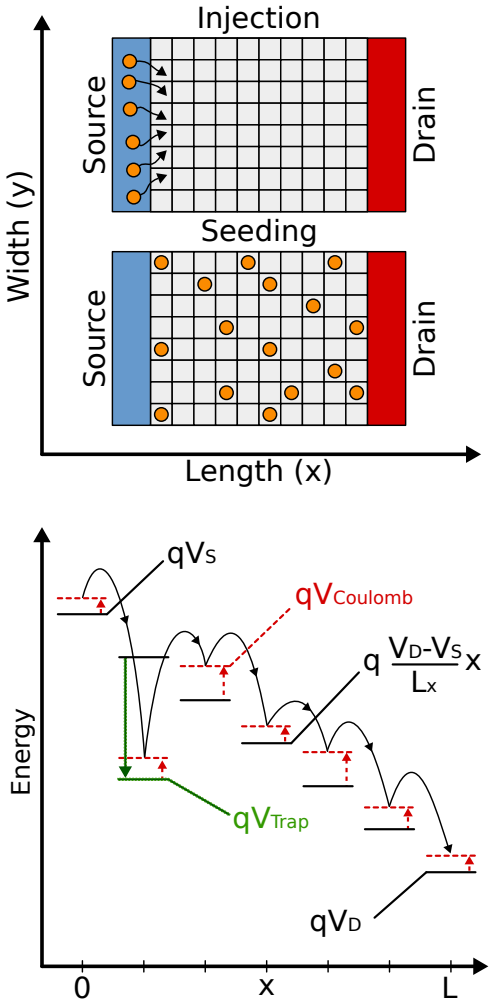
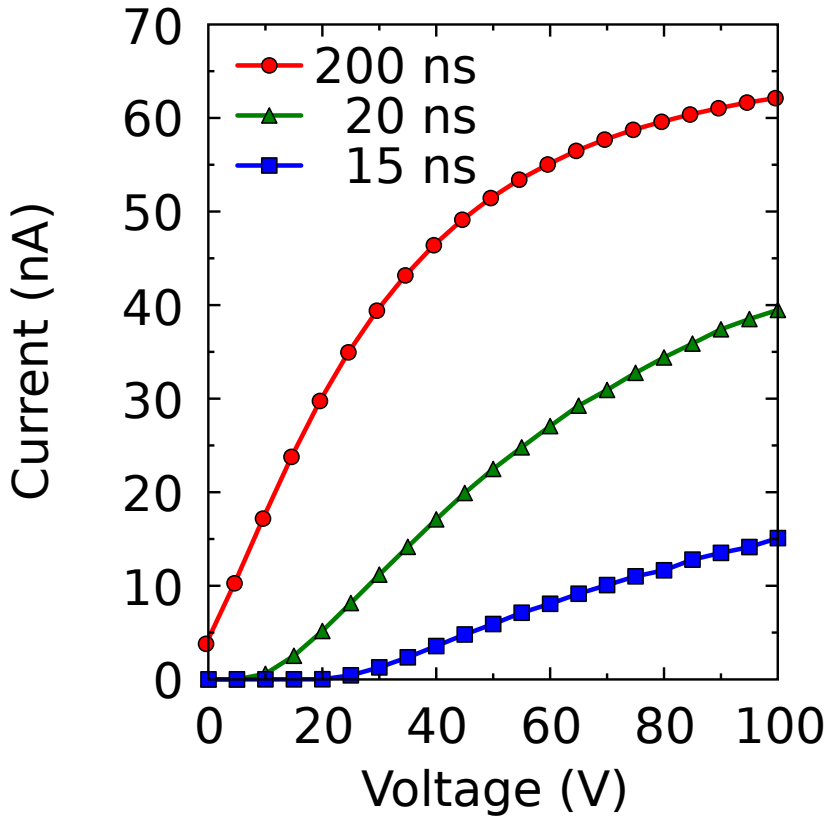
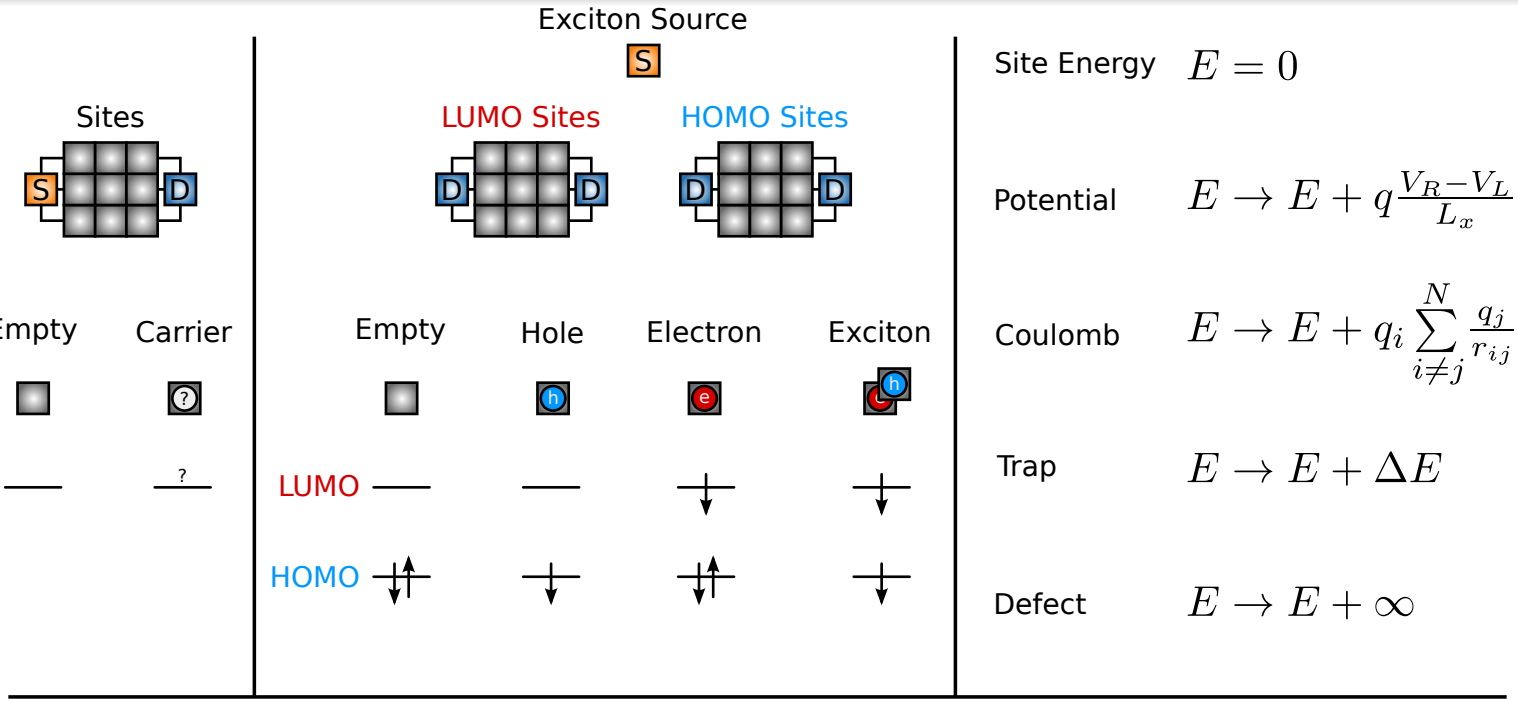
Langmuir (OFET Model)



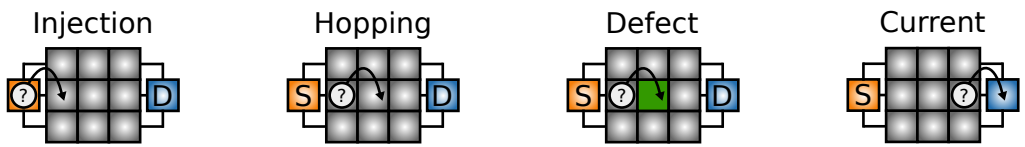


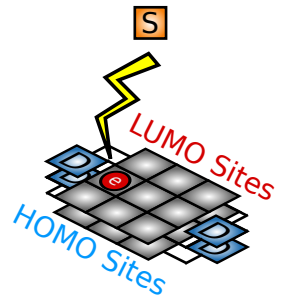
Langmuir (OFET Model and OPV Model)



$P_{acc} = min\left[1, e^{-\frac{\Delta E}{kT}}\right]$

$P_{acc} = constant$





$P_{acc} = constant$

$P_{acc} = 0$

$P_{acc} = constant$

Monte Carlo

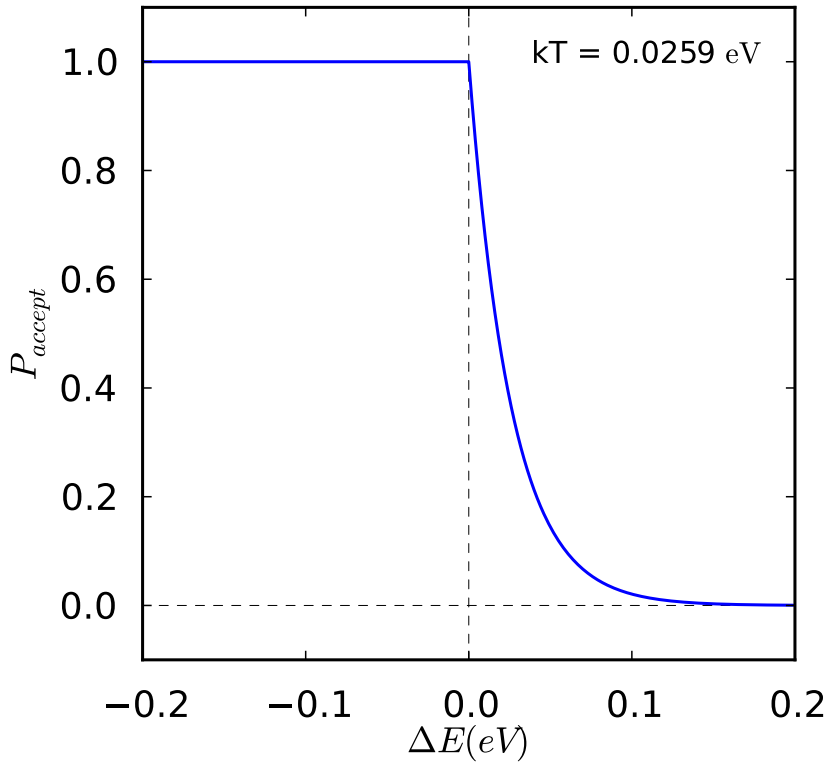
$$P^{old\to new}_{propose} \times P^{old\to new}_{accept} \times P_{old} = P^{new\to old}_{propose} \times P^{new\to old}_{accept} \times P_{new}$$

$$P^{old\to new}_{propose} = P^{new\to old}_{propose}$$

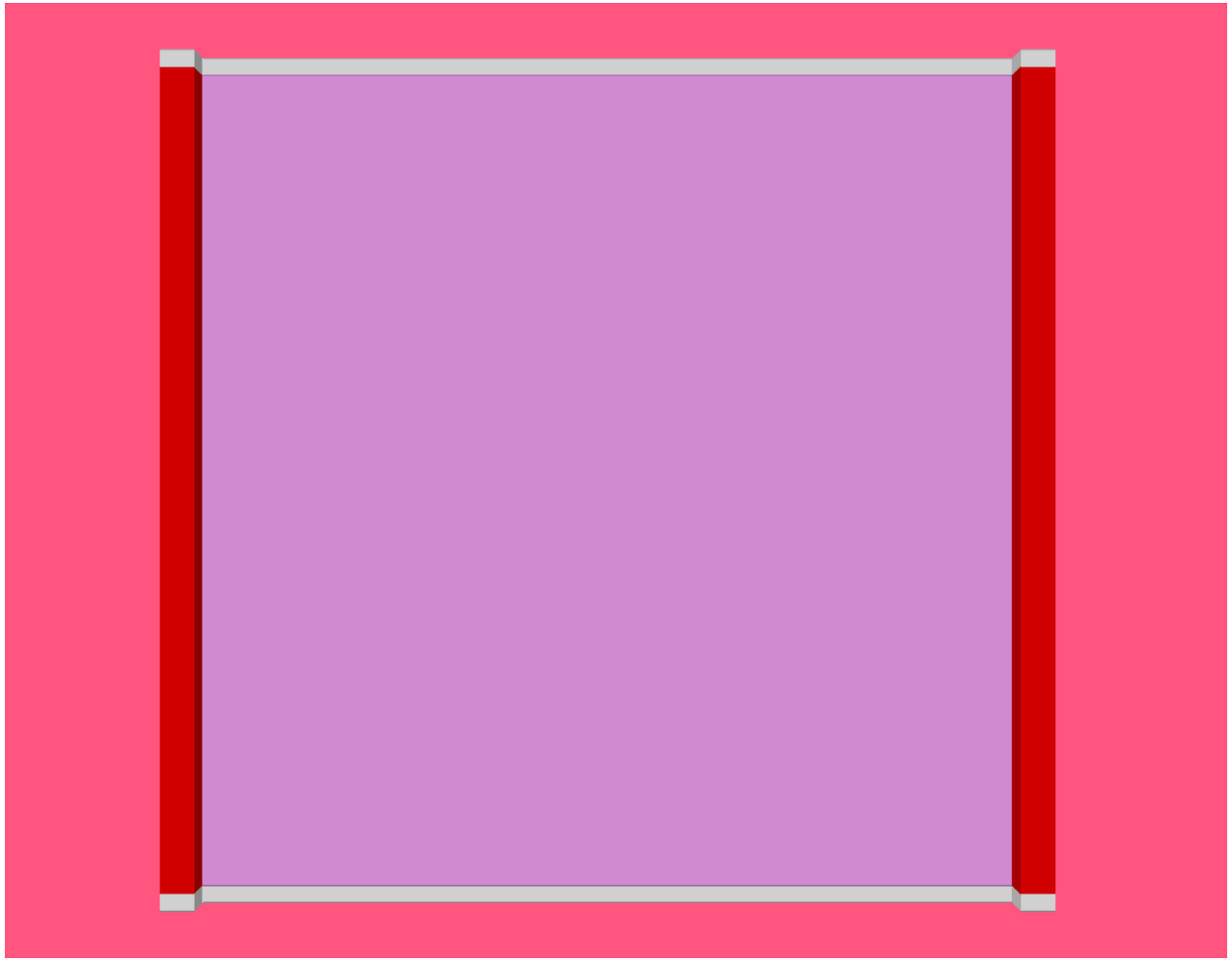
$$P_{old} \propto e^{\frac{-E_{old}}{kT}}$$

$$P_{new} \propto e^{\frac{-E_{new}}{kT}}$$

$$P^{old\to new}_{accept} = min\left[1.0, e^{\frac{-(E_{new}-E_{old})}{kT}}\right]$$



Movie



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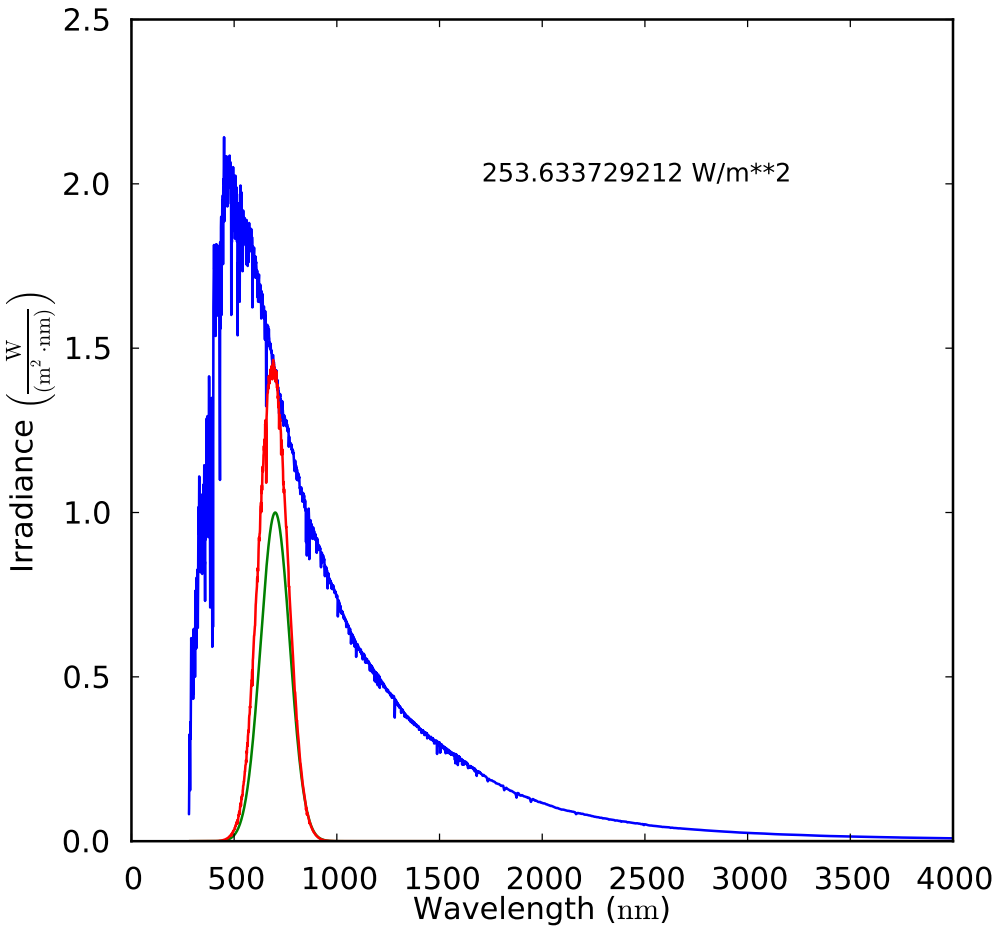
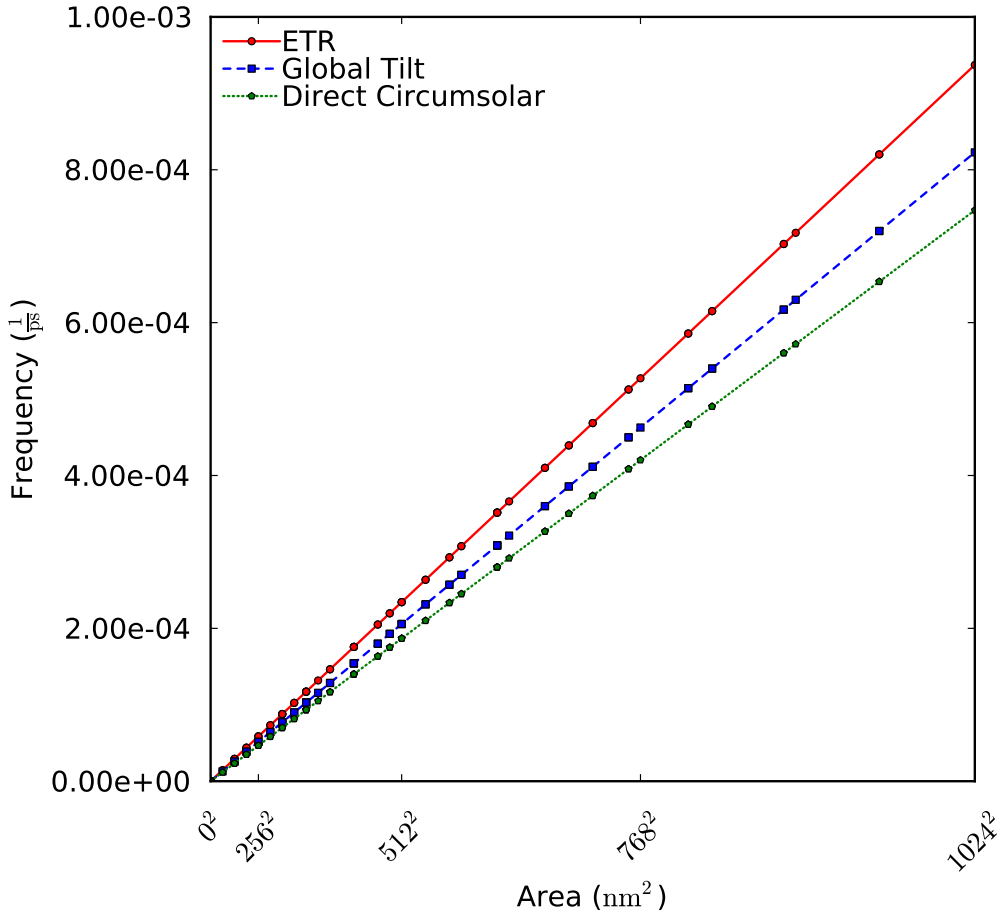
AM1.5 (Estimating Injection Rate)

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



AM1.5 (Estimating Injection Rate)

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



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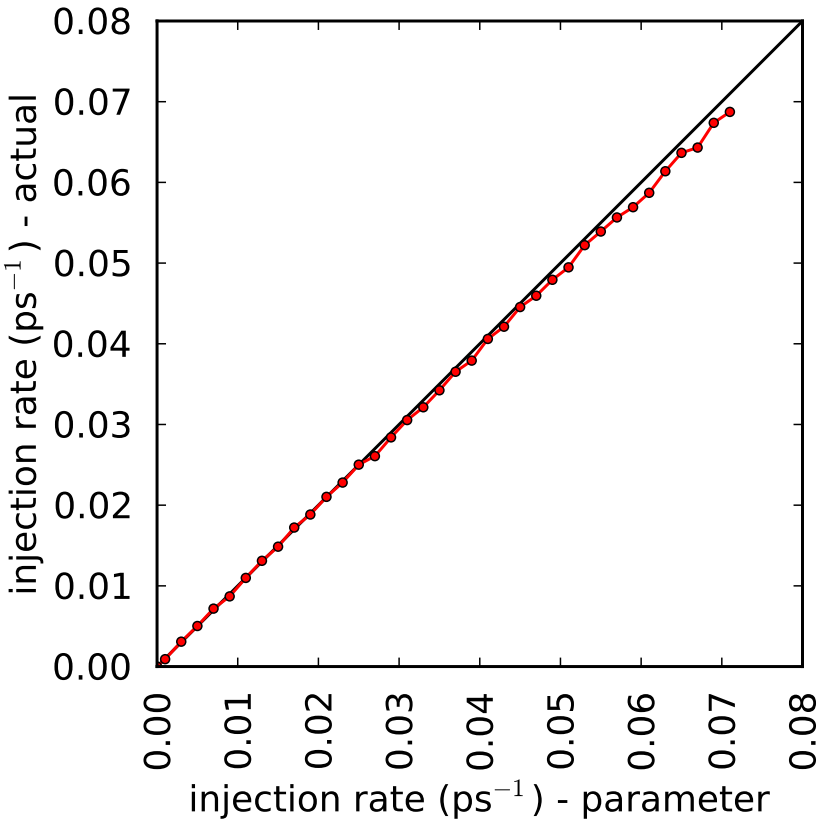
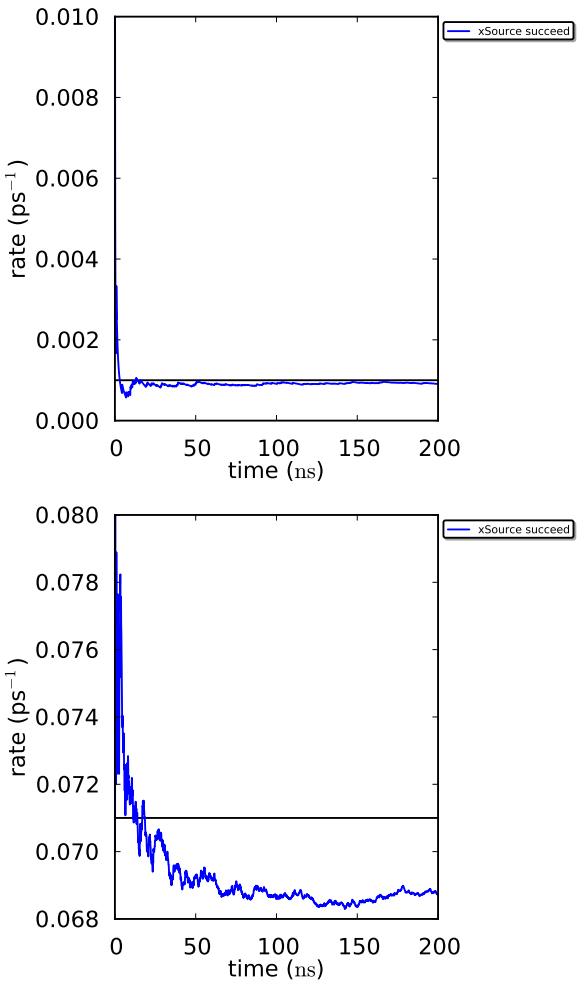
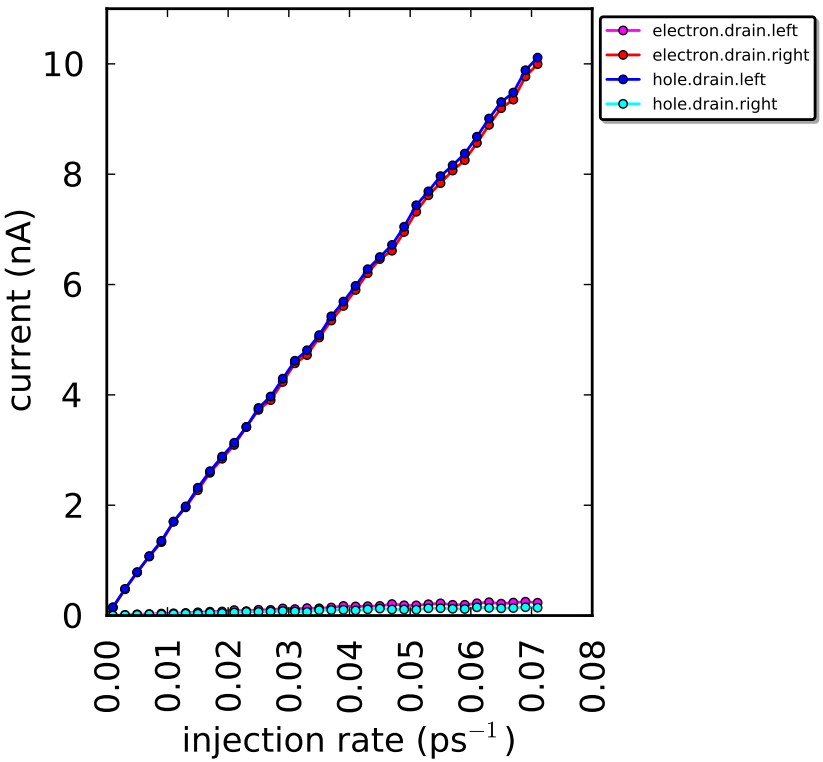
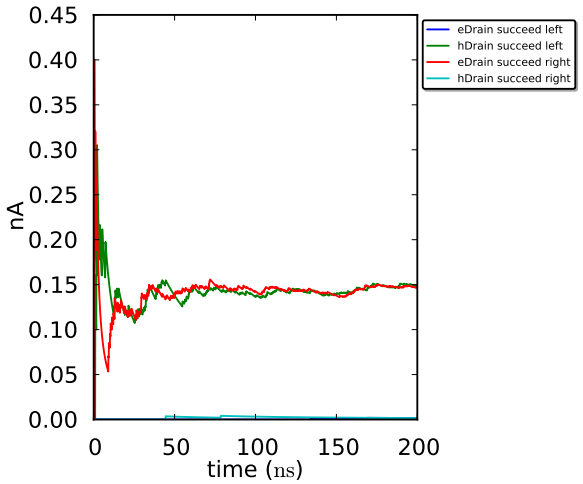
Exciton Injection Rate

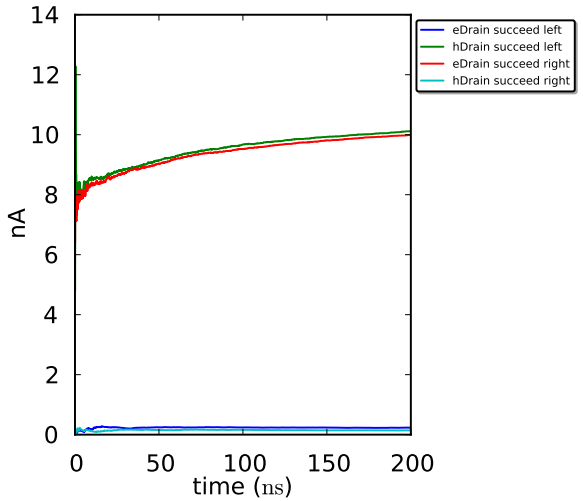




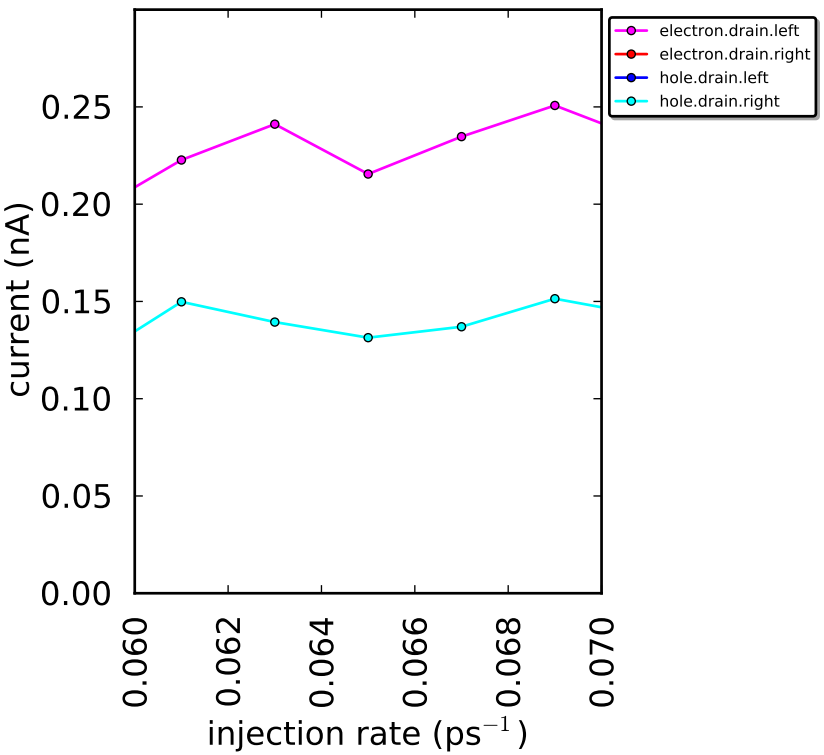
Current at the Electrodes

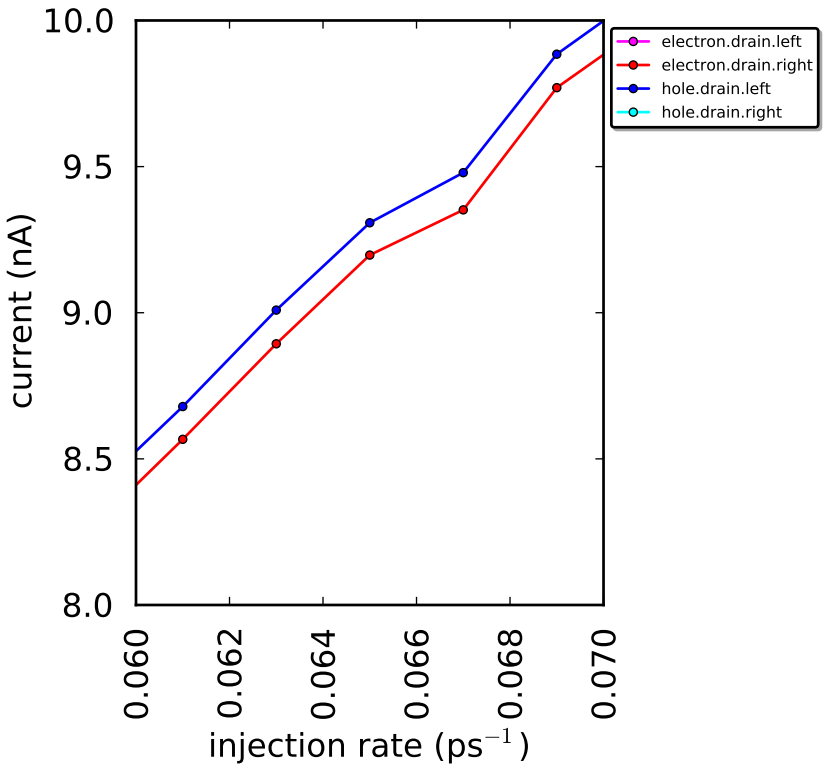




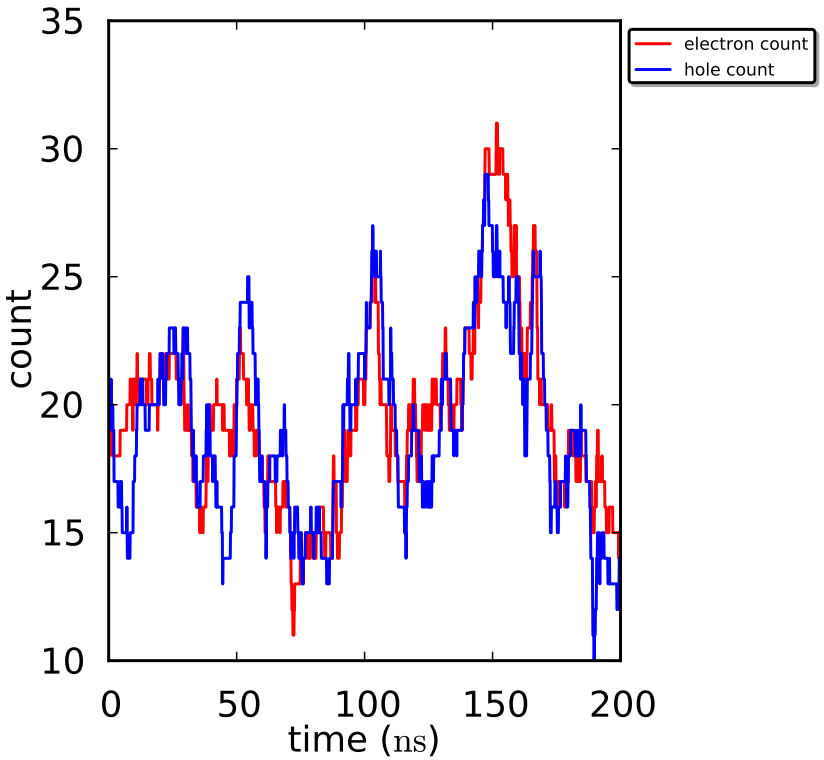


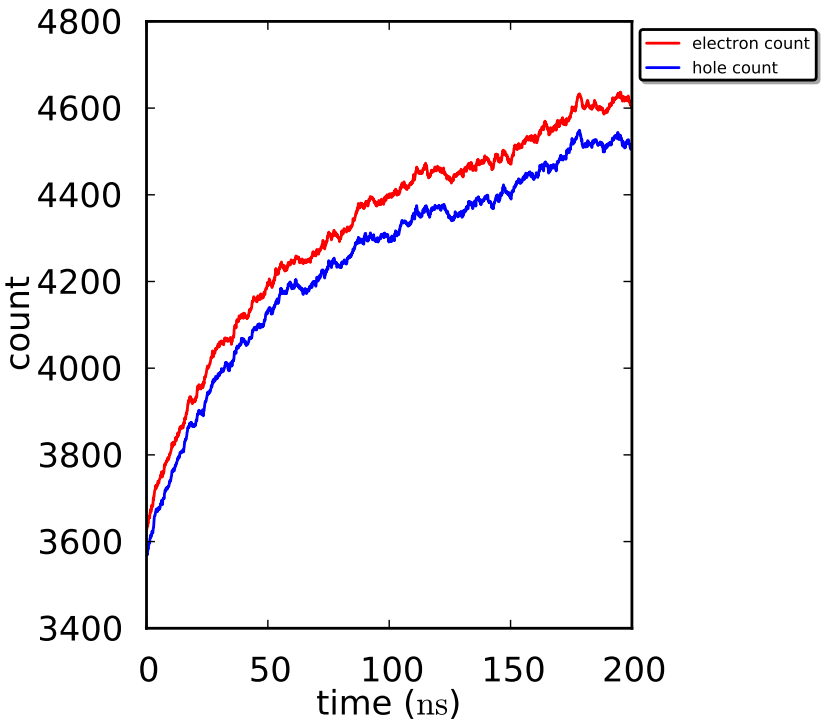
Current at the Electrodes Zoomed In





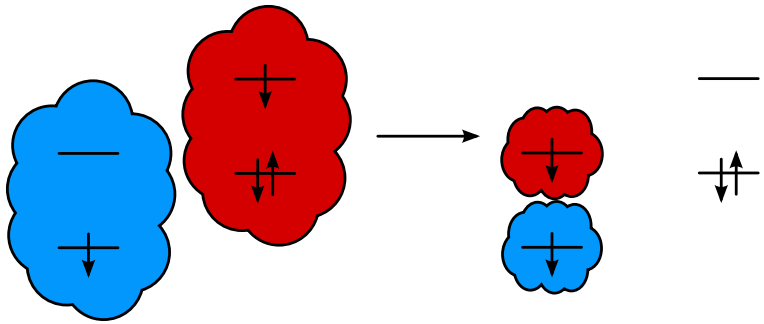
Charge Imbalance?





Thoughts on Imbalance

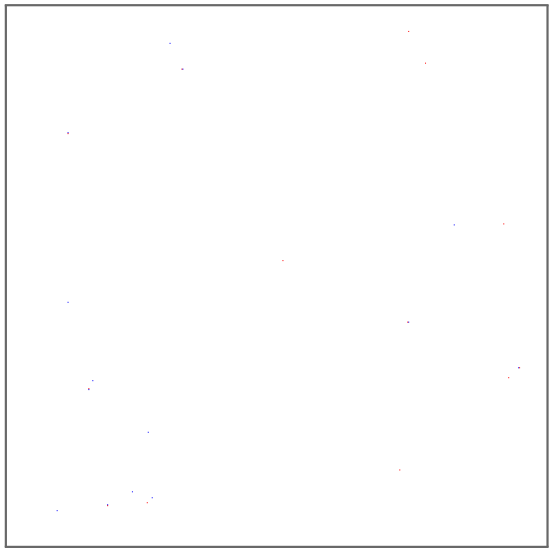
$$\frac{q_i q_j}{r_{ij}} = 0 \quad @ \quad r_{ij} = 0$$

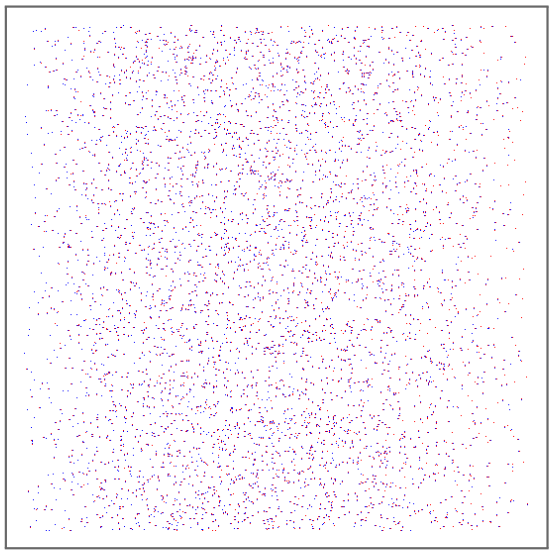


$$E = ... + \frac{-e^2}{1} \qquad E = ... + 0$$

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

$$E_{Coulomb} += contant;$$





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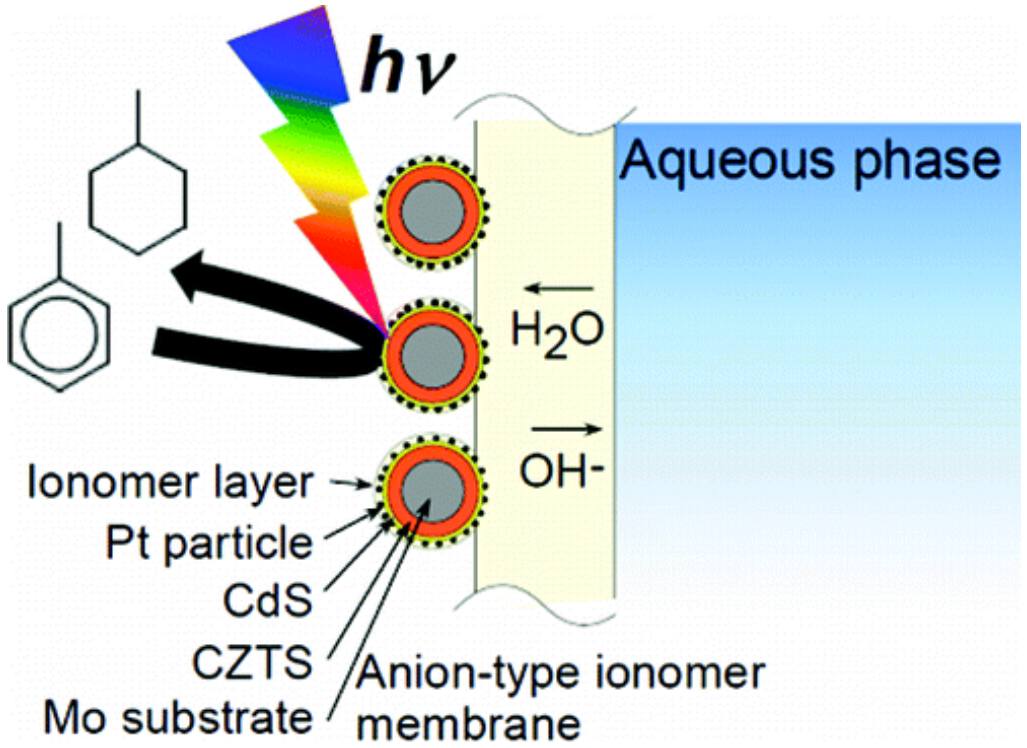
Questions?



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