The impact of intra sub-band tail states on charge carrier trapping and collection in organic solar cells

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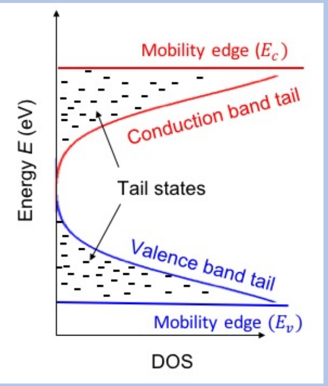
1. Introduction: localised tail states

Organic semiconductors used in optoelectronic devices are not ideal as a result of the disorder in molecular conformation (orientations of the molecular backbone), intermolecular interactions, and the presence of chemical or other defects. This disorder results in intra sub-band energy states lying between the conduction and valence bands.



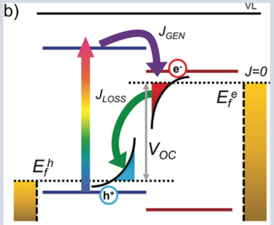
The tail states distribution can be described by exponentially decay towards the bandgap (similar distribution to Gaussian) below the band edge.

$$N_{CBT} = N_{0CBT}\exp\left(\frac{E-E_C}{E_{chC}}\right)$$

$$N_{VBT} = N_{0VBT}\exp\left(\frac{E-E_V}{E_{chV}}\right)$$

These intra sub-band tail states are functional for charge transport and recombination to different degrees, depend on its **density** and **shape** (distribution).

2. Experimental method: charge extraction (CE)



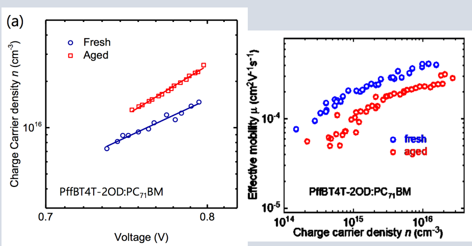
Using a charge extraction experiment, a solar cell is held at a certain light and voltage bias before the light bias is switched off at the same time as the voltage is switched to short circuit.

$$n_{CE} = n_0\exp(\gamma V_{oc})$$

$$n_{ave} \propto \exp\left(\frac{E_f}{2E_{ch}}\right),$$

Tail states slope: when $V_{OC} = E_f$, $\gamma = \frac{1}{2E_{ch}}$

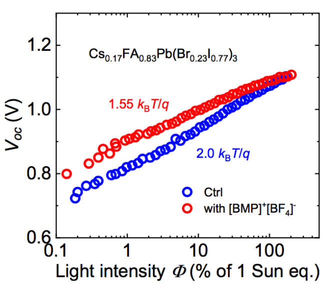
3. Impact of tail state density on charge carrier transport



The burn-in process induced the formation of additional intra bandgap states, causes more severer charge trapping and leads to reduced charge carrier mobility.

H. Cha, J. Wu, A. Wadsworth, J. Nagitta, S. Limbu, S. Pont, Z. Li, J. Searle, M. F. Wyatt, D. Baran, J.-S. Kim, I. McCulloch and J. R. Durrant, *Adv. Mater.*, 2017, **29**, 1701156.

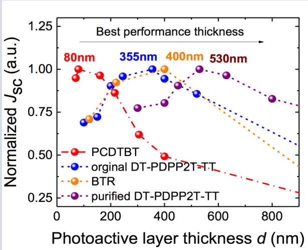
4. Correlation between V_{OC} dependence and tail states distribution

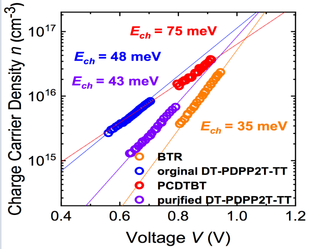


$$R \propto n_{free}p_t \propto \exp\left(\frac{\Delta E_f}{2kT}\right)\exp\left(\frac{\Delta E_f}{2E_{ch}}\right) = \exp\left(\frac{\Delta E_f}{kT}\left(\frac{1}{2}+\frac{kT}{2E_{ch}}\right)\right)$$

Y. Lin, N.Sakai, P. Da, J. Wu et al. Science (2020)

5. Photocurrent collection in thick devices





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