Device Model Study of Dark Injection in Organic Semiconductors

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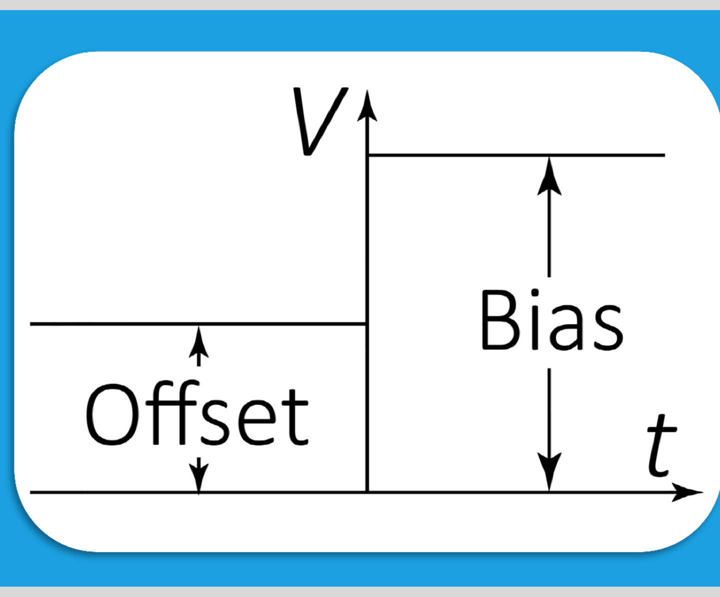
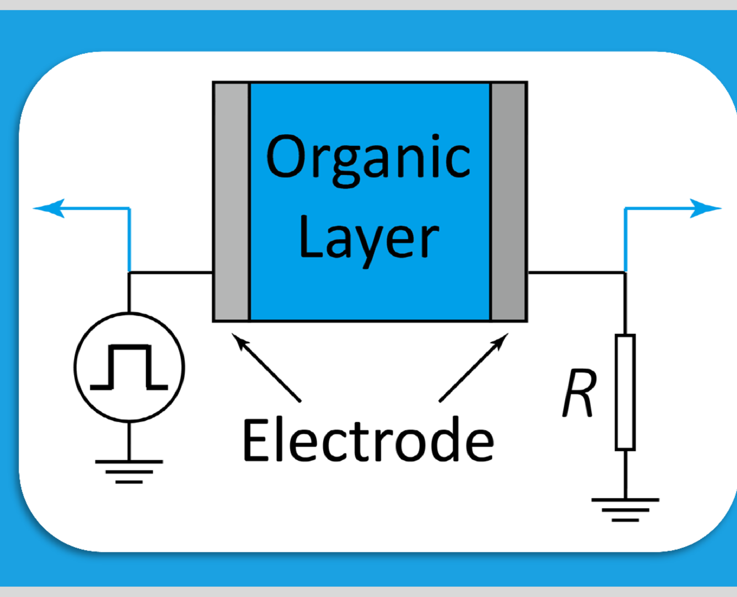
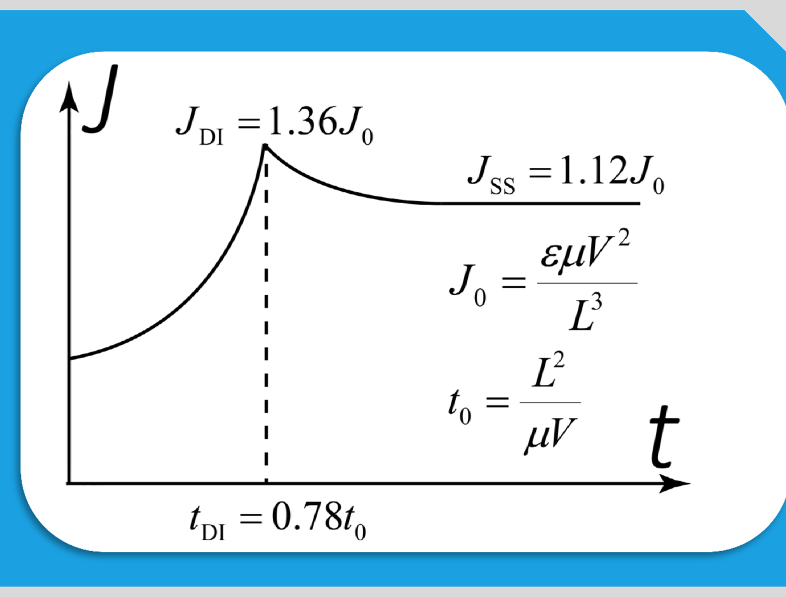
I. Introduction: Measuring Mobility

- Mobility: Characteristic of organic semiconductors
- Dark injection (DI): current response to a step voltage [1]

Technique	Merits	Limits
Time of flight	Optical generation	Thick film
Dark injection	Thin-films compatible	'Ohmic' contact







II. *t*-Dependent Device Model

- Continuity equation

$$\frac{\partial p}{\partial t} + \frac{1}{e}\frac{\partial J_p}{\partial x} = G - R$$

$$\frac{\partial n}{\partial t} - \frac{1}{e}\frac{\partial J_n}{\partial x} = G - R$$

- Drift-Diffusion current

$$J_p = e\mu_p\left(pE - \frac{k_B T}{e}\frac{\partial p}{\partial x}\right)$$

$$J_n = e\mu_n\left(nE + \frac{k_B T}{e}\frac{\partial n}{\partial x}\right)$$

- Poisson equation

$$\frac{\partial E}{\partial x} = \frac{e}{\varepsilon}(p - n)$$

- Trap-Releasing equation

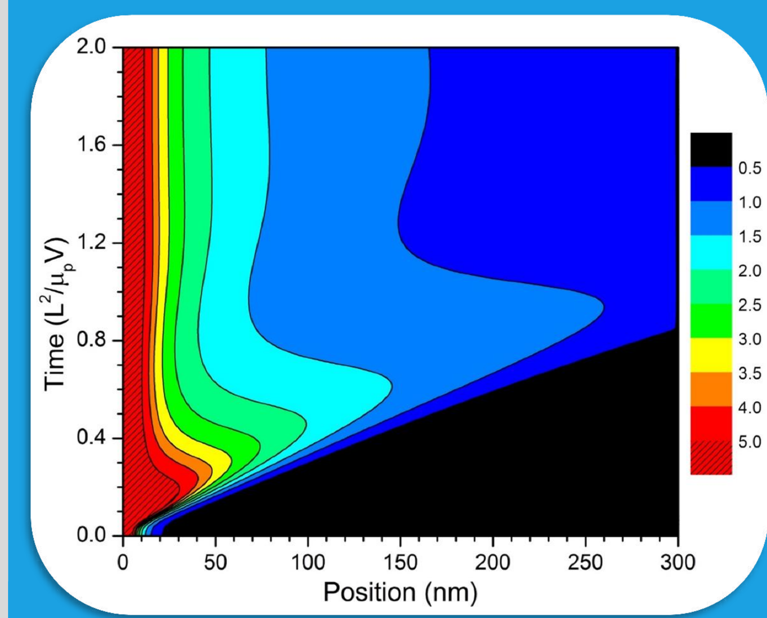
$$\frac{\partial p_t}{\partial t} = r_t p (N_t - p_t) - r_r p_t$$

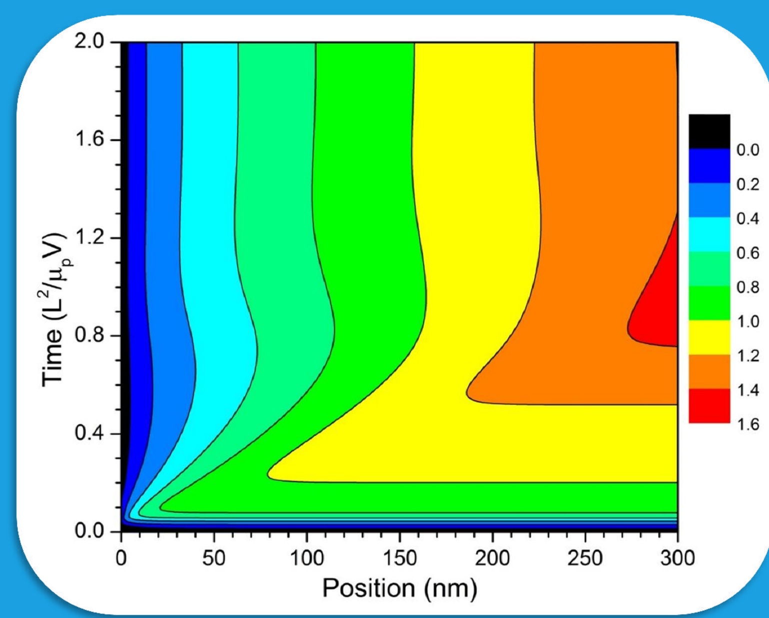
- Recast of Poisson equation for the dynamics

$$\frac{\partial E}{\partial t} = \frac{1}{\varepsilon}\left[-(J_p + J_n) + \frac{1}{SR_{ext}}\left(V - |V_{bi}| - \int_0^L E\,dx\right)\right]$$

p/n	Density (Hole/electron)	N_t	Trap density
$J_{p/n}$	Electric current	$r_{t/r}$	Kinetic coefficients
$\mu_{p/n}$	Mobility	S	Device area
E	Electric field	R_{ext}	Circuit resistance
V_{bi}	Built-in potential	p_t	Trap charge density
G/R	Generation/Recombination		

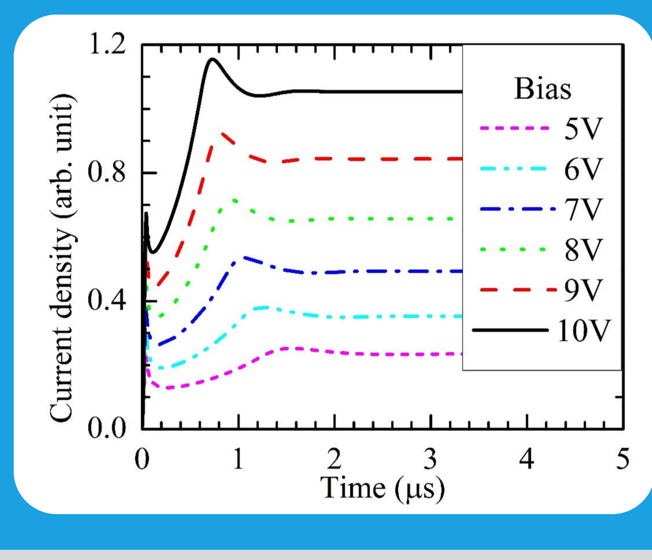
III. Physical Processes

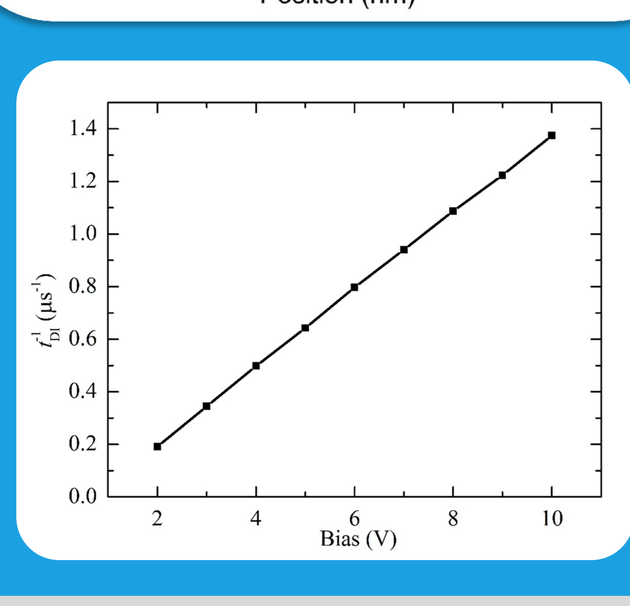




Evolution of physical quantities

- Charge density (left) and electric field (right)
- Space charges (holes) from the anode with the step voltage arrive at the cathode roughly at t_{DI}.
- Instead of monotonic relaxation to steady state, the field at the cathode shows a maximum.
- There are enough space charges to disturb the field, leading to space-charge-limited current.

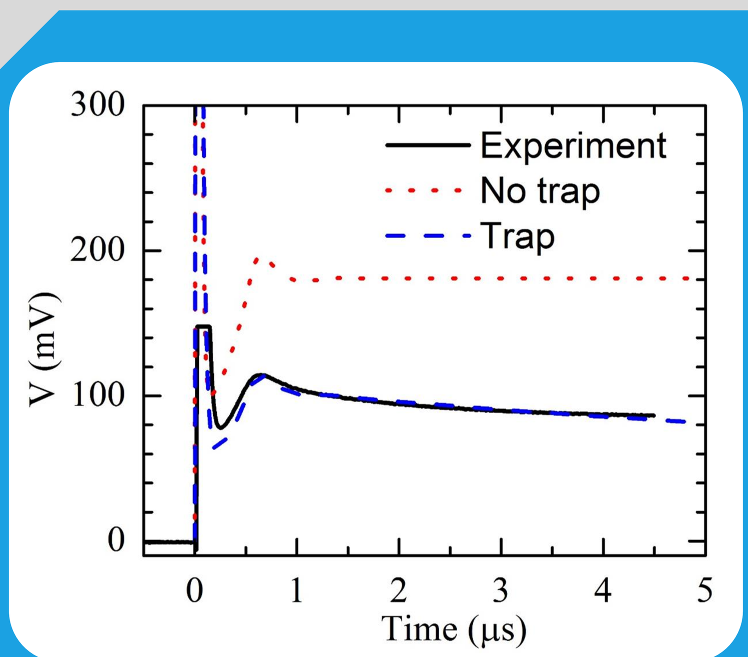


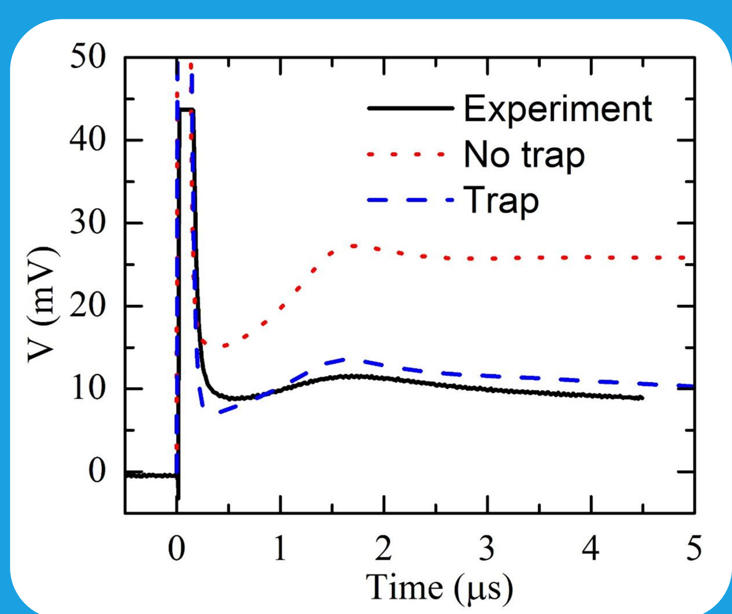


Typical simulation results

- Left: DI transients with offset 0 and varying bias
- Right: inverse t_{DI} *vs* bias.
- The DI transients become clearer with increasing bias, due to more space charges injected.
- The linear relation between inverse t_{DI} and bias is got in correspondence with analytical results.

IV. Modeling the Experimental Results



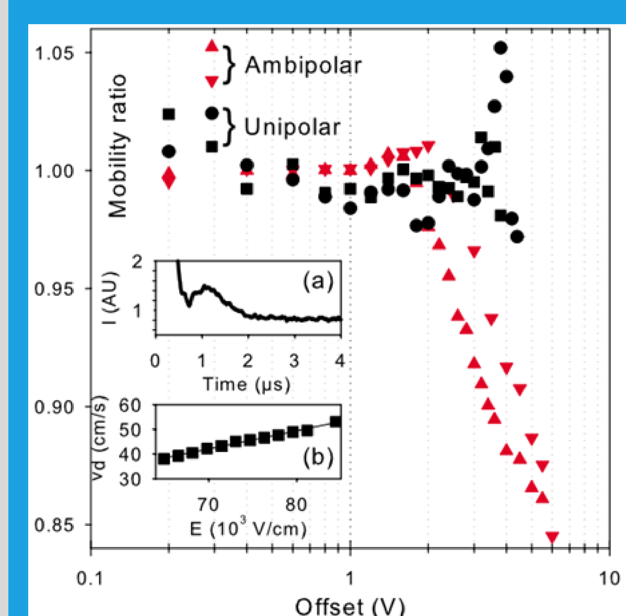


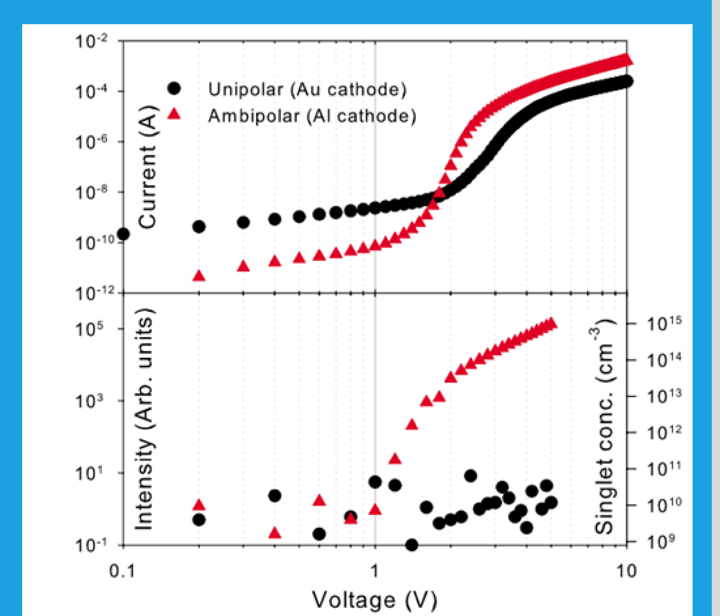
DI transients at 10V (left) and 5V (right) with parameters for TPD

- Experimental DI transients of TPD can be simulated with realistic parameters.
- The signal is the voltage drop across the circuit resistance.
- Traps are essential, which cause the decaying tail of the transients.

V. Mobility Ratio (MR)

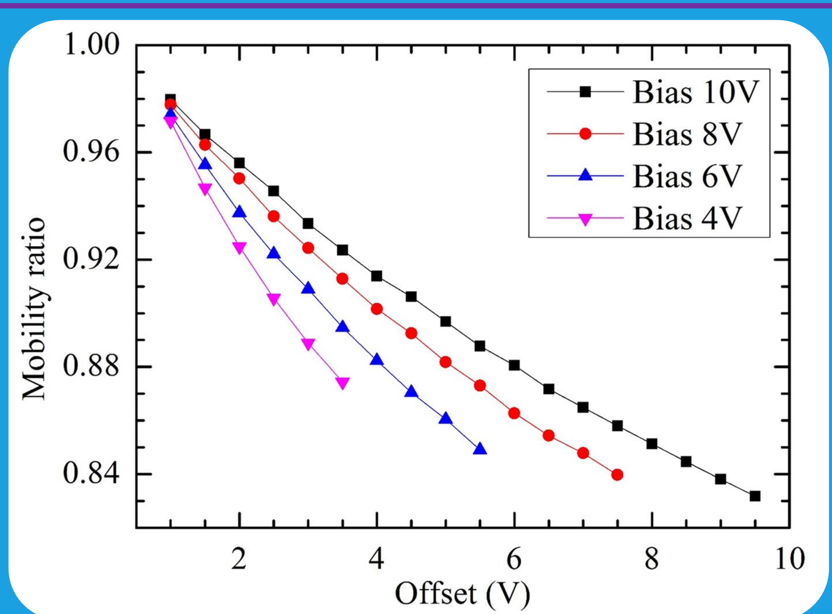
- A new application of DI transients is to study the change of the peak position with an offset, reflected by the MR $\mu(\text{offset})/\mu_0$.
- Experiments have shown that the MR remains constant (decreases) in unipolar (bipolar) devices. [2]
- The contrast is attributed to the blocking of charge carriers by triplet excitons in bipolar device.





The J-V and EL-V curve (left) and mobility ratio (right) of a TPD device reported in [2].

VI. Puzzle of the Mobility Ratio



MR *vs* offset with different bias

- However, the space-charge injected by the offset screens part of the field at the anode. The charges injected by the step voltage feels a smaller field, resulting in a larger t_{DI}. The MR should decrease even in unipolar devices.
- The constant MR is itself a puzzle to the device model, let alone the reason of the MR drop in bipolar one.
- Future: clarify the role of screening in organic semiconductors

VI. Conclusions, Acknowledgement and References

We study the dark injection transients in organic semiconductors with the time-dependent device model. The current takes the drift-diffusion form and the traps are explicitly considered. The simulation captures both the peak and the decay of the dark injection signal. The scale of the peak position with carrier mobility is also obtained. The mobility ratio is calculated with an initial offset voltage and the results show discrepancy with experimental observations. This calls for clarification of the actual role of the screening effect in organic semiconductors.

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[1] A. Many and G. Rakavy Phys. Rev. **126**, 1980 (1962).
[2] J. Y. Song, N. Stingelin, A. J. Drew, T. Kreouzis, and W. P. Gillin Phys. Rev. B **82**, 085205 (2010).

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