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Charge-carrier relaxation in disordered organic semiconductors studied by dark injection and impedance spectroscopy

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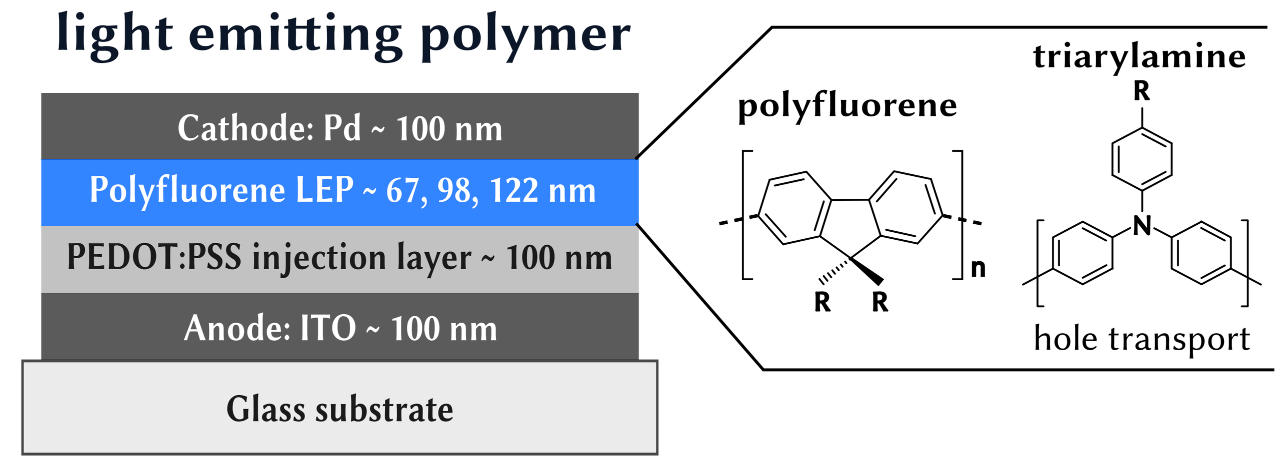
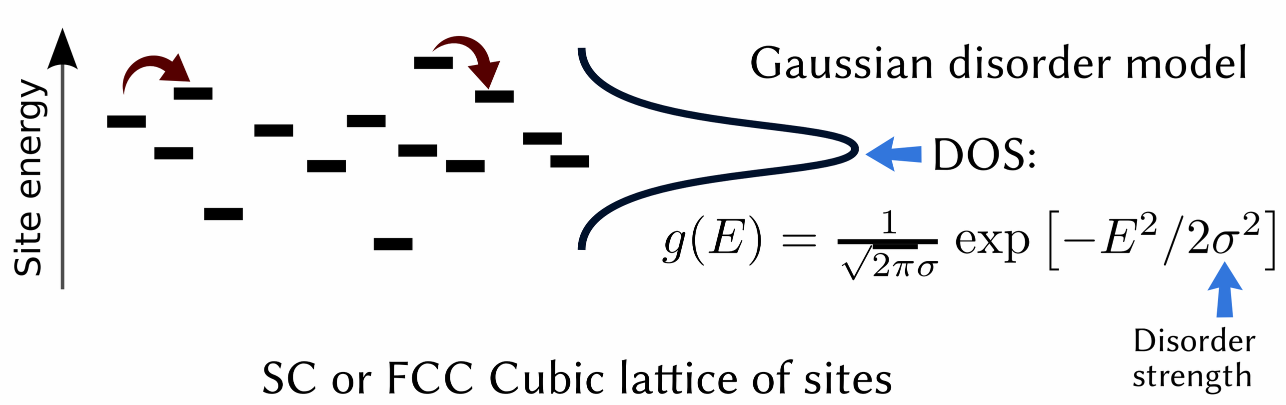
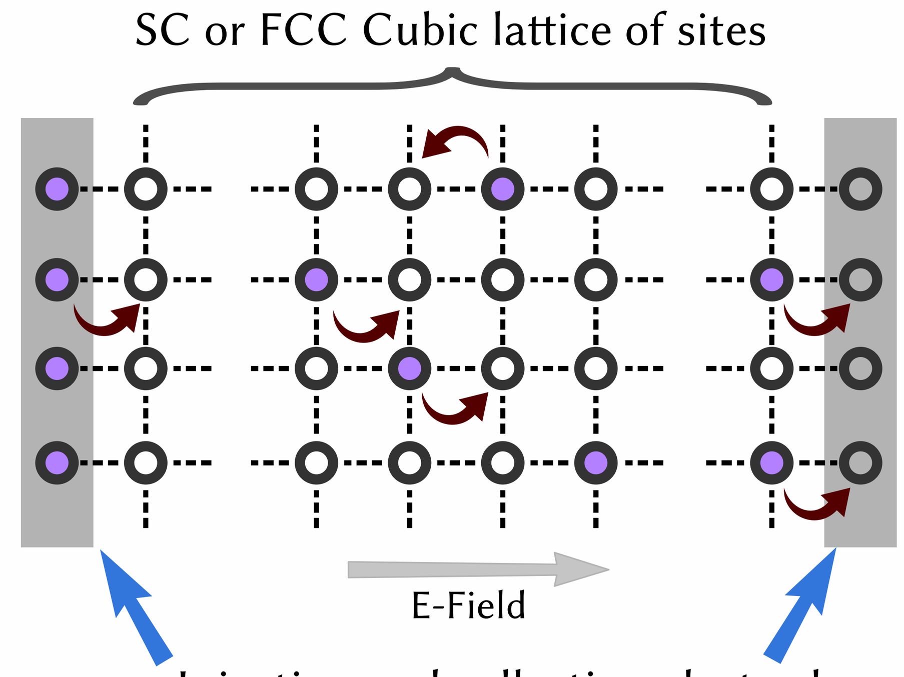
Understanding of stationary charge transport in disordered organic semiconductors has matured during recent years. However, charge-carrier transport in non-stationary situations is still poorly understood. Such relaxation can be studied in dark injection and impedance spectroscopy experiments. The resulting transient current and low-frequency capacitance-voltage profile reveal both charge-carrier transport and relaxation characteristics. We performed such experiments on hole-only devices of a polyfluorene-based organic semiconductor. The modelling has been done by solving time-dependent master equation in the framework of the Gaussian disorder model.

Hole transport in blue light emitting polymer



Numerical methods





Miller-Abrahams hopping:

$$W_{ij} = \nu_0 \exp(-2\alpha R_{ij}) \times \exp\left[-(\Delta E_{ij} - |\Delta E_{ij}|)/2k_B T\right]$$

Intrinsic hopping rate; Inverse wavefunction localization length; hopping distance; energy difference

3D master-equation model

$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = \sum_{j \neq i} \left[W_{ji} p_j (1-p_i) - W_{ij} p_i (1-p_j)\right]$$

time-dependent cccupational probability

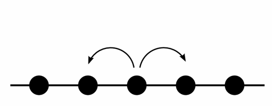
p_i's are calculated by a combination of Newton's method and implicit Euler method at each time step.

$$J(t) = \frac{e}{L L_y L_z} \sum_{i,j} W_{ij} p_i (1-p_j) R_{ij,x} + \frac{\epsilon_0 \epsilon_r}{L} \frac{\mathrm{d}V}{\mathrm{d}t}$$

Device thickness; Single-bond current; Displacement current

1D master-equation model

Linear chain of discrete sites

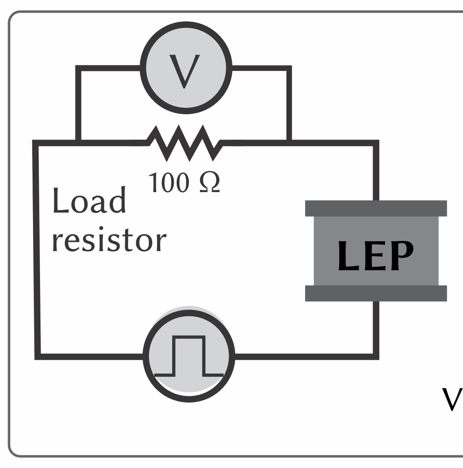


Computationaly convenient but no carrier relaxation effects!

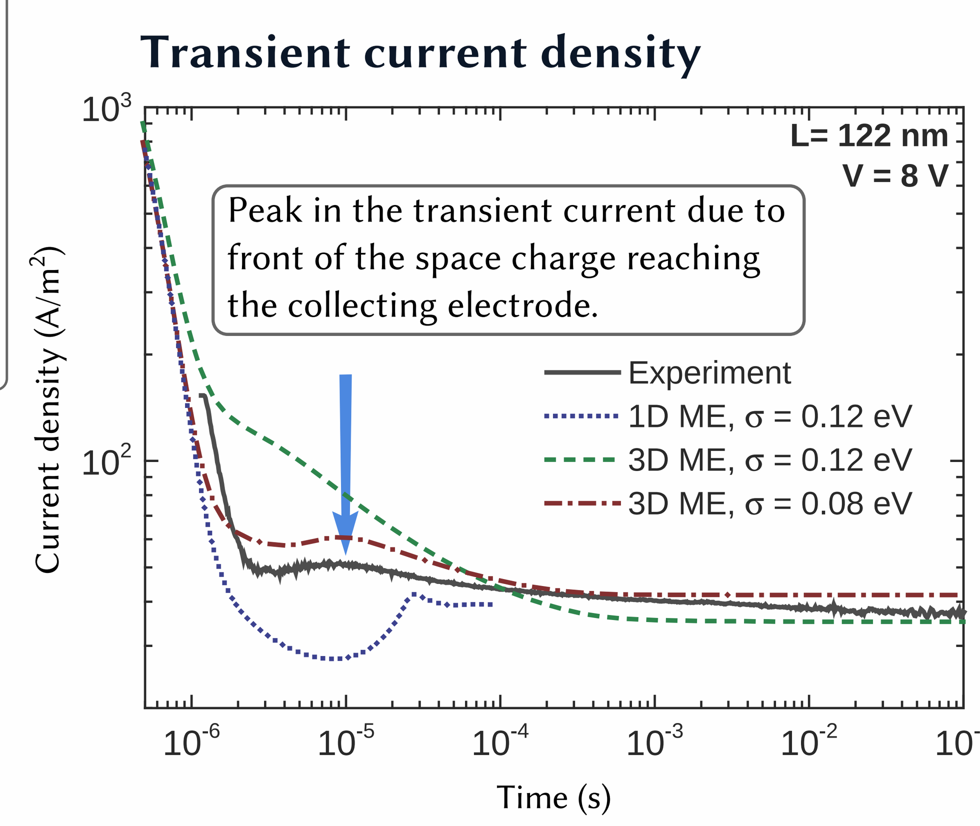
$$\frac{\mathrm{d}c_i}{\mathrm{d}t} = c_{i-1} r_i^+ + c_{i+1} r_{i+1}^- - c_i (r_{i+1}^+ + r_i^-)$$

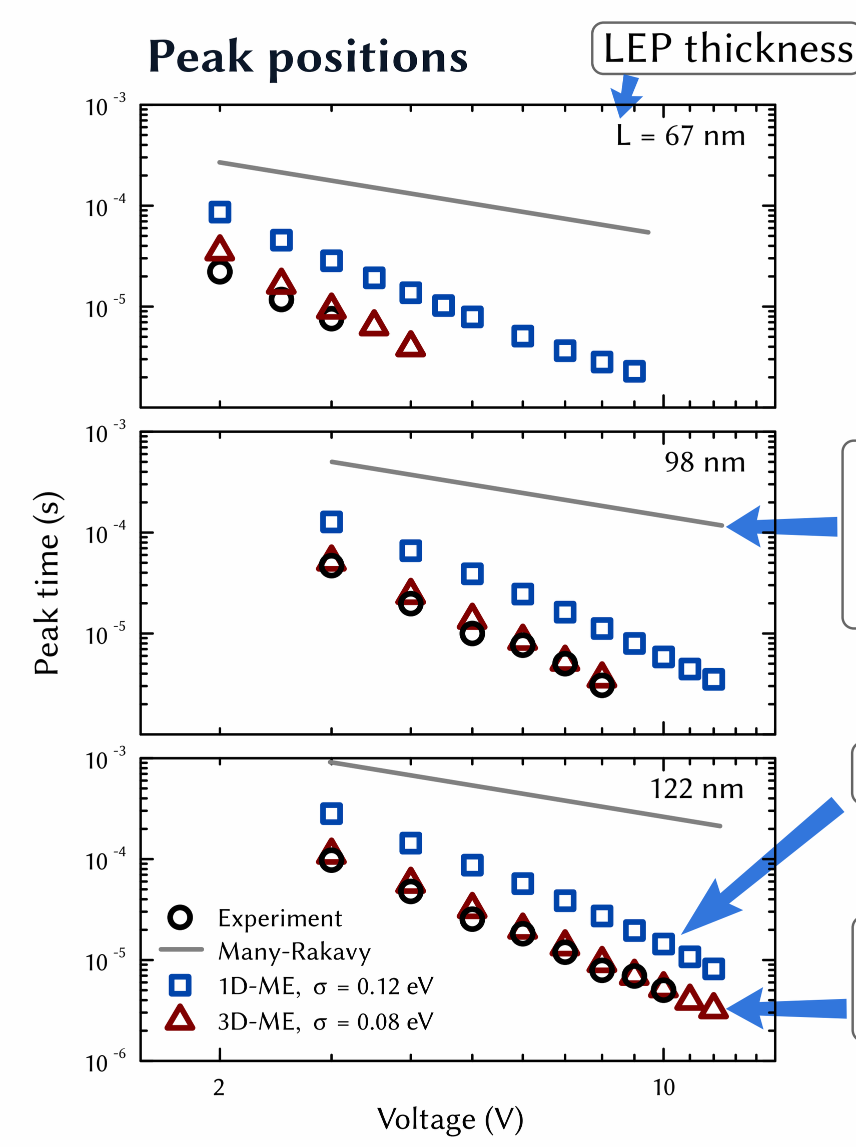
Carrier concentration; Forward, backward hops

Dark injection transient current



Transient current is monitored when the voltage is abruptly increased.





Many-Rakavy: *Phys. Rev.* **126** 1980

$$t_{\mathrm{peak}} = 0.786 \frac{L^2}{\mu V}$$

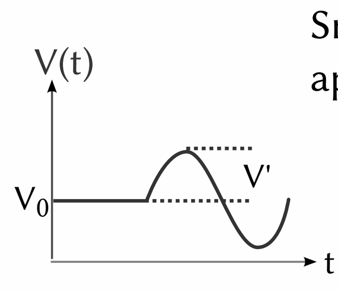
Peak is more pronounced with smaller disorder strength!

No charge-carrier relaxation

Nice agreement with the experiment when charge-carrier-relaxation effects are considered!

Low-frequency capacitance by impedance spectroscopy

Small amplitude ac-signal is applied to a pre-biased sample



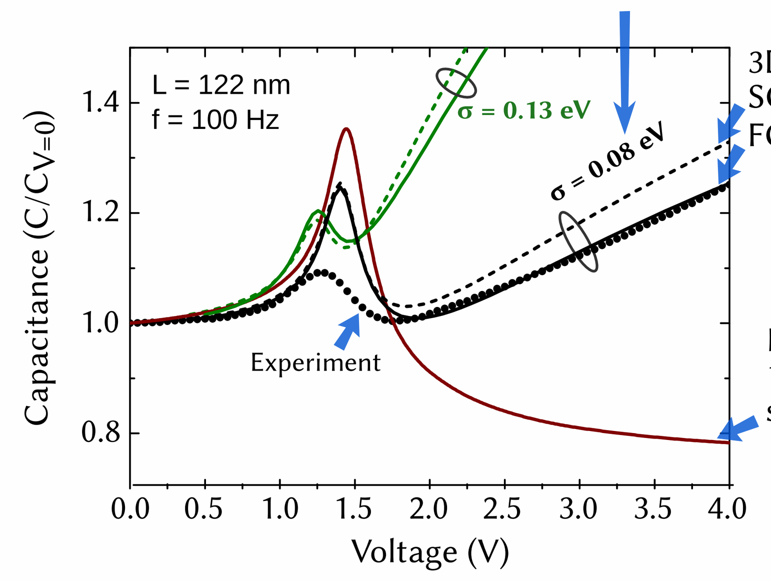
$V_0 \gg V'$

$V(t) = V_0 + V' \sin(2\pi i f t)$ (Frequency)

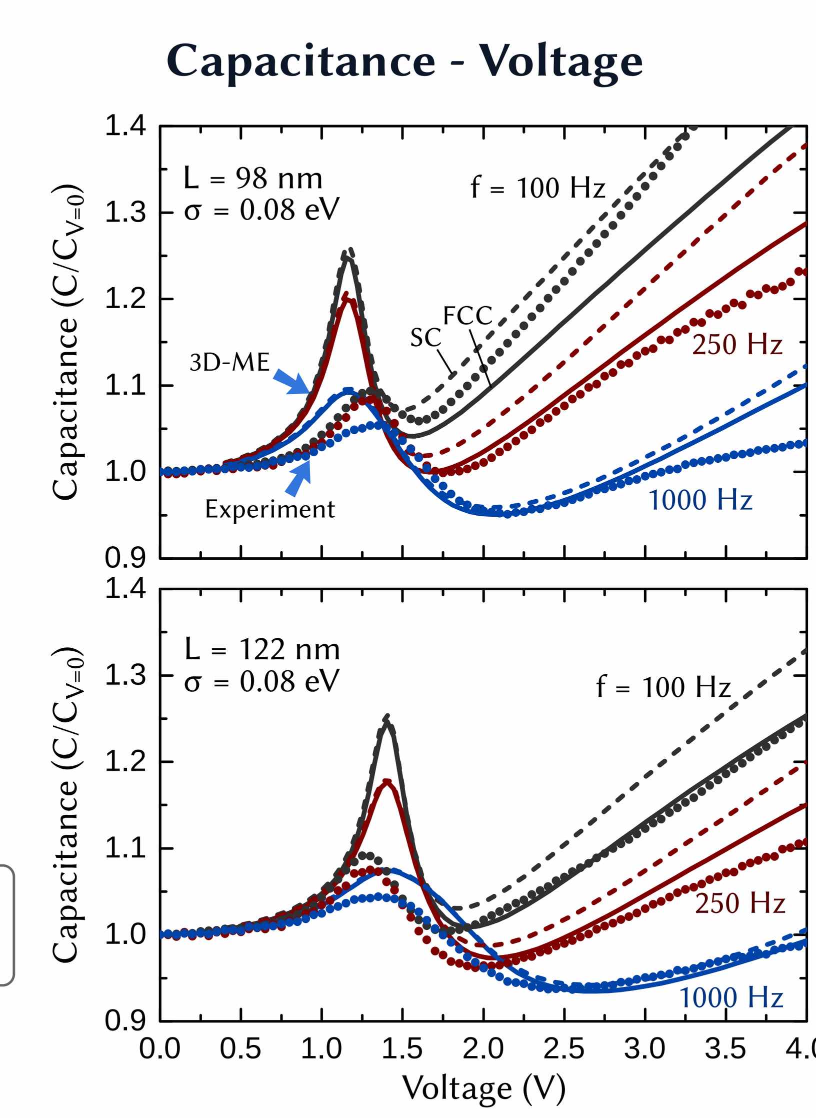
$Z = Z' + iZ''$, $C = -Z''/2\pi f |Z|^2$

Impedance; Capacitance

3D-ME simulations: smaller σ than obtained from steady-state current-voltage fits, gives better agreement with experiment.



Type of lattice has a minor influence



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