

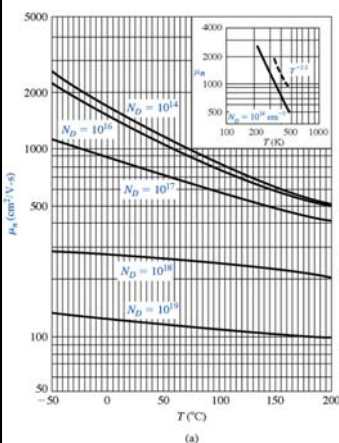
# 전자물리특강: Charge Transport in Organic Semiconductors

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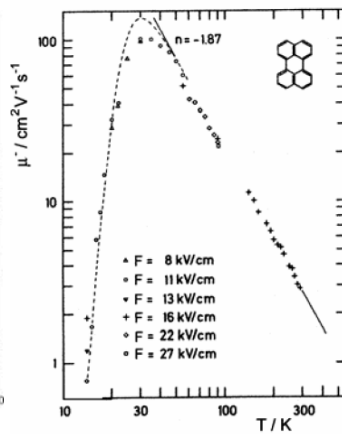


## Carrier mobility of Si and Organic Materials

Electron mobility of Si

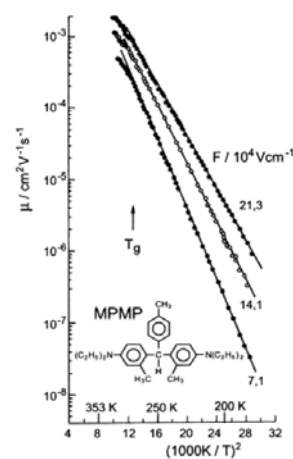


Electron mobility of Perylene



370 nm thick perylene crystal

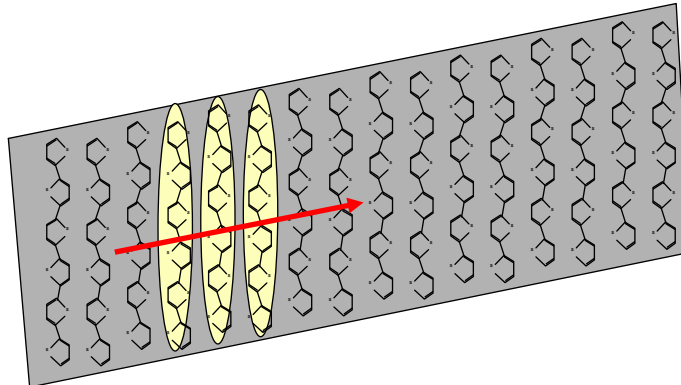
Electron mobility of MPMP



8.7  $\mu$ m thick unordered layer of MPMP (sublimed).



- Van der Waals forces hold molecules together
- Charge hopping, the major factor limiting mobility, takes place from molecule to molecule
- Phonons help electrons hop, therefore increasing mobility
- Mobility increases with temperature because of phonons

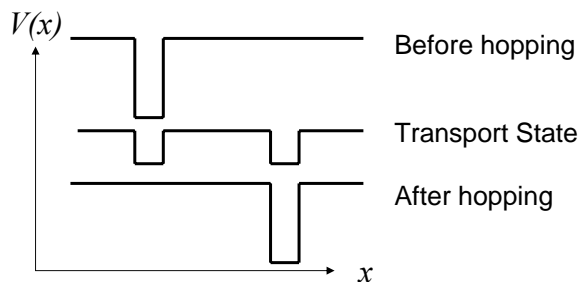


## Why Localized States?

- 1) Polaron formation
- 2) Disorder (energetic and structural disorder)

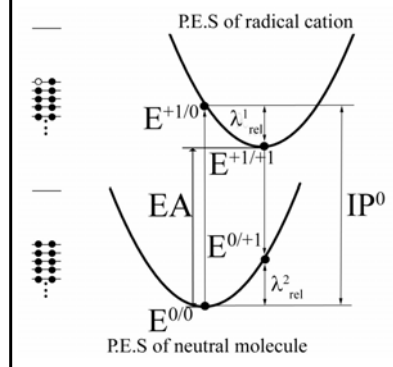
### 1) Polaron

- Charge carrier lowers its energy by lattice distortion
- Strong electron-lattice (phonon) interaction leads to self-localisation
- The rate of charge transfer is limited by the reorganization of the molecules.



electron - transfer (hopping) rate,  $k_{ET}$

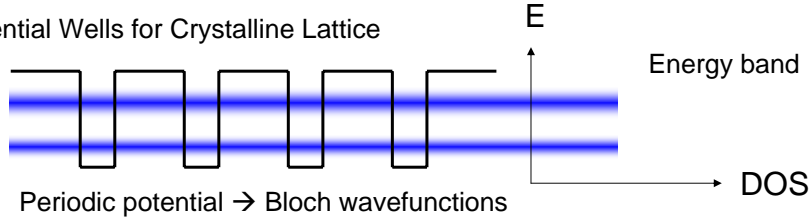
$$k_{ET} = A \cdot \exp\left[-\frac{(\lambda - 2t)^2}{4\lambda k_B T}\right]$$



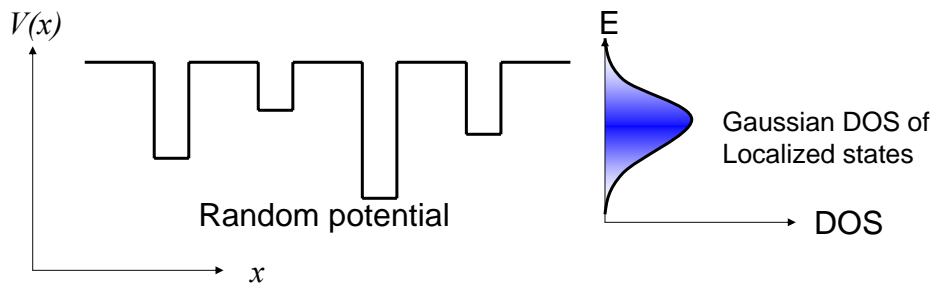
## 2) Disorder

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- Potential Wells for Crystalline Lattice



- Sufficient disorder produces localized states (P. W. Anderson)



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## Hopping = phonon-assisted tunneling

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- Carriers tunnel directly from one localized state to another when the electronic wave functions of the defect states have sufficient overlap.
- The carrier can overcome the energy differences between the defect states by absorbing and emitting phonons.

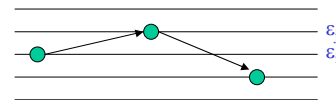


Ref. E.M. Conwell, Phys. Rev. 103 (1956) 51.

N.F. Mott, Can. J. Phys. 34 (1956) 1356; N.F. Mott, E.A. Davis, Electronic Processes in Noncrystalline Materials, Clarendon Press, Oxford, 1971.

- The transition rates for phonon-assisted tunneling (Miller and Abrahams):

$$W_{ij} = v_{ph} \exp(-2\alpha R_{ij}) \begin{cases} \exp(-\frac{\epsilon_i - \epsilon_j}{kT}), & \epsilon_i > \epsilon_j \\ 1, & \epsilon_i < \epsilon_j \end{cases}$$



$\alpha$  = inverse localization length,  $R_{ij}$  = distance between the localized states,  $\epsilon_i$  = energy at the state  $i$ .

- Since the hopping rates are strongly dependent on both the positions and the energies of the localized states, hopping transport is extremely sensitive to structural as well as energetic disorder.

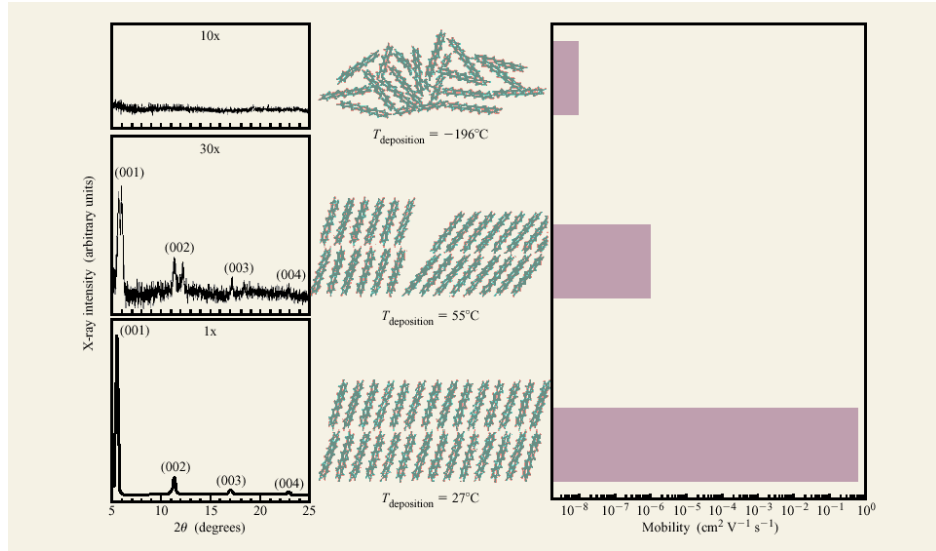
Ref. A. Miller, E. Abrahams, Phys. Rev. 120 (1960) 745.

B.I. Shklovskii, A.L. Efros, Electronic Properties of Doped Semiconductors, Springer, Berlin, 1984.



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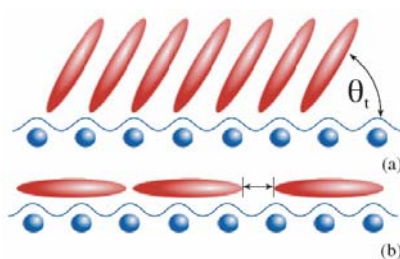
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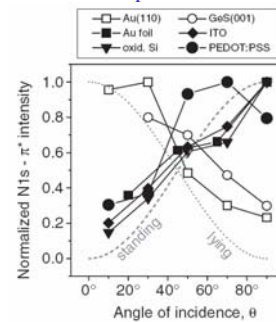
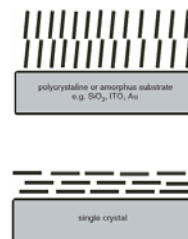
J. M. Shaw, P. F. Seidler, *IBM J. Res. & Dev.*, 45, 3 (2001)



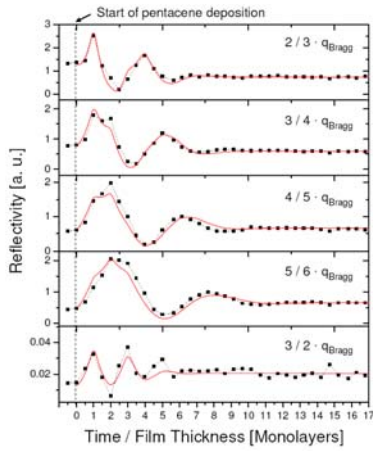
1. Organic molecules are 'extended objects' and thus have internal degrees of freedom (vibrational, conformational, and orientational). This is probably the most fundamental difference between growth of atomic and growth of organic systems.
2. The size of the molecules and the associated unit cells are greater than that of typical (inorganic) substrates.
3. The interaction potential (molecule-molecule and molecule-substrate) is generally different from the case of atomic adsorbates, and van-der-Waals interactions are more important.



F. Schreiber, *phys. stat. sol. (a)* 201, No. 6, 1037–1054 (2004)



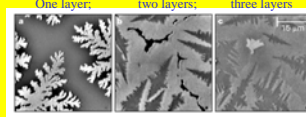
Growth on a SiO<sub>2</sub>/Si wafer at 50 °C



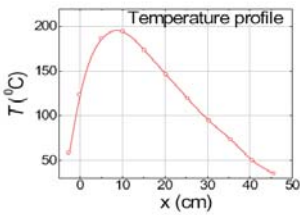
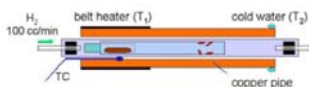
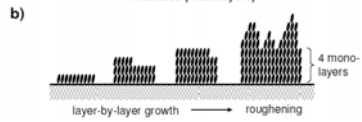
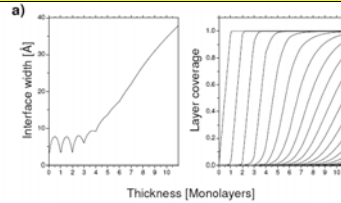
Pentacene growth exhibits a marked transition from layer-by-layer growth to strong roughening after a thickness of about four pentacene (mono-) layers.

S. Kowarik, A. Gerlach, W. Leitenberger, J. Hu, G. Witte, C. Wöll, U. Pietsch, and F. Schreiber, *Thin Solid Films* (2007).

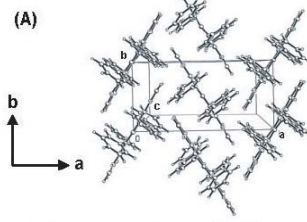
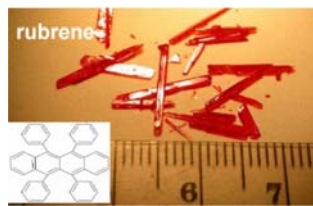
Development of the pentacene layer-by-layer contrast during deposition on Si(001) during growth at a rate of 10<sup>-2</sup> monolayers per minute (one monolayer (ML) ~15 Å).



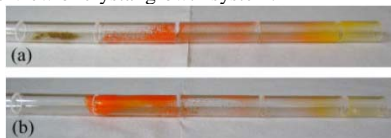
F.-J. M. z. Heringdorf, M. C. Reuter and R. M. Tromp, *Nature* **412**, 517-520 (2001)



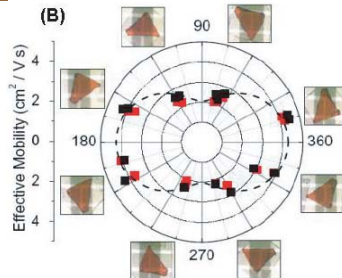
The angular dependence of the mobility for a rubrene crystal, measured at room temperature.



Schematic overview of crystal growth system.

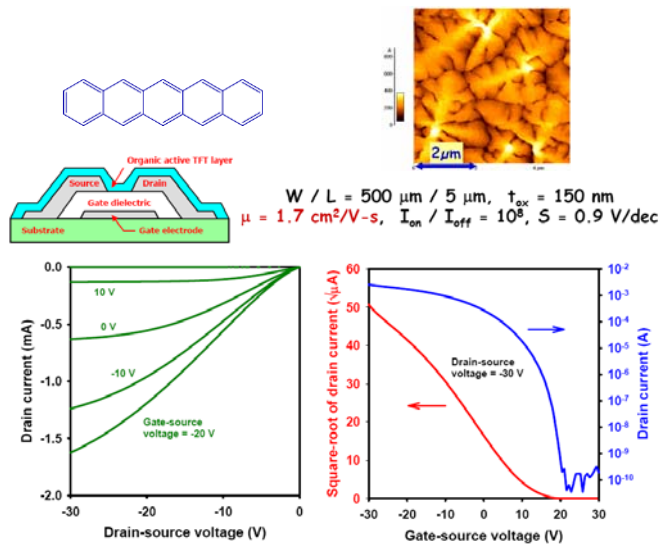
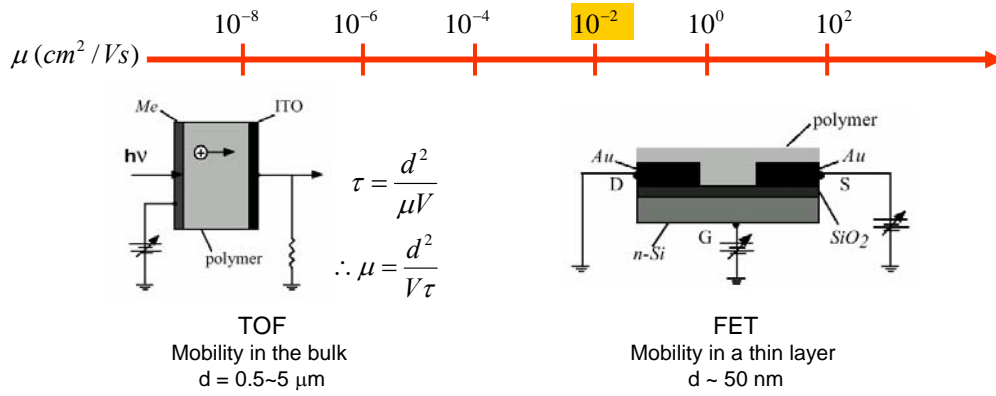


(a) Result after first regrowth of as-purchased organic material.  
(b) At the end of the second regrowth no dark residue is present at the position of the source material, which demonstrate the purifying effect of the growth process.



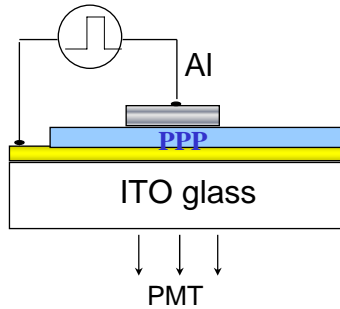
R. W. I. de Boer, M. E. Gershenson, A. F. Morpurgo, and V. Podzorov, *phys. stat. sol. (a)* **201**, No. 6, 1302-1331 (2004).





# Transient EL

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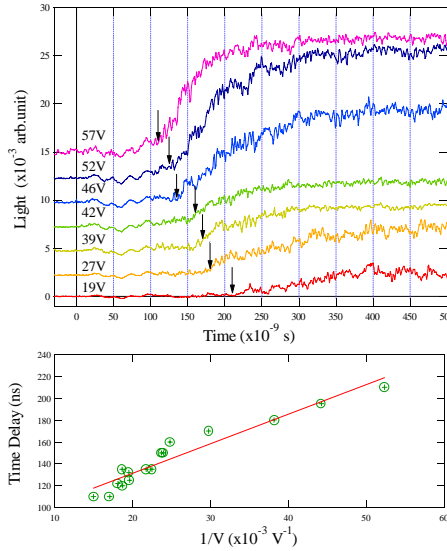
Mobility from the delay time

$$\tau = d^2 / \mu V$$

Hole mobility

in the vacuum-deposited PPP:

$$\text{ITO/PPP/Al: } \mu = 4.5 \times 10^{-6} \text{ cm}^2/\text{Vs}$$

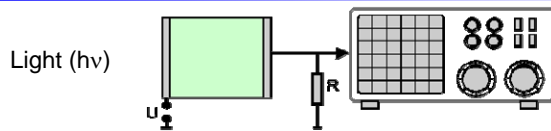


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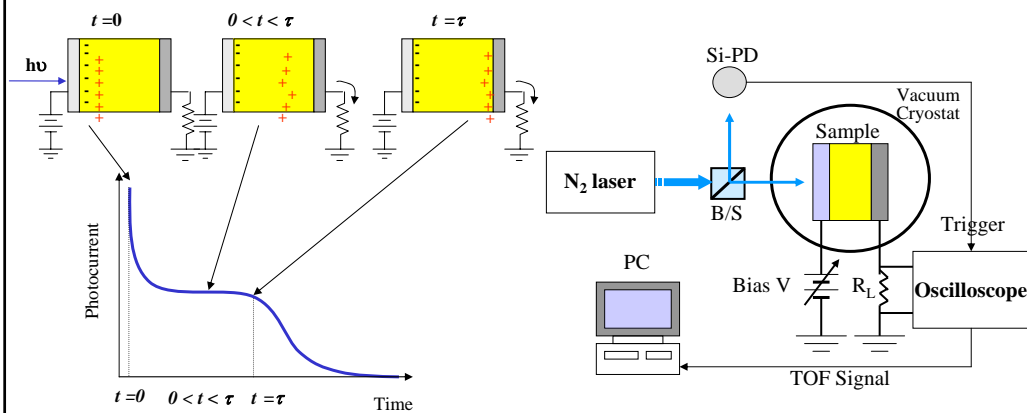
# TOF-PC

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$$\mu = \frac{d^2}{V\tau}$$

Time-of-flight photoconductivity

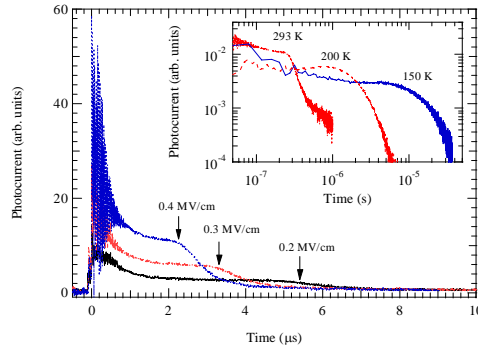
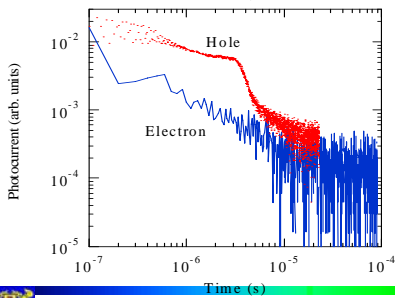
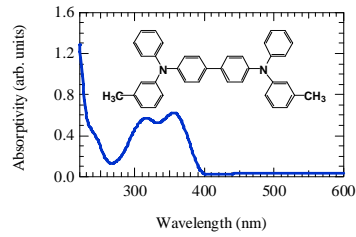
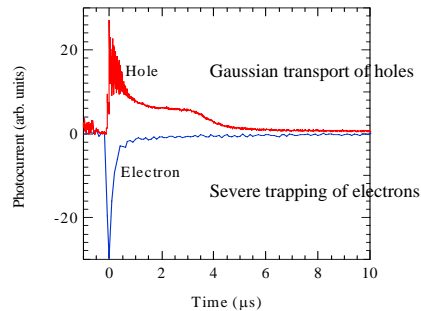


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# TOF-PC Signals of TPD

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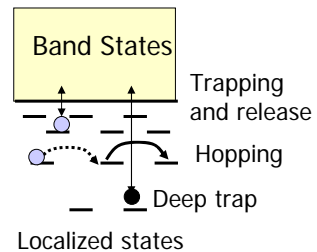
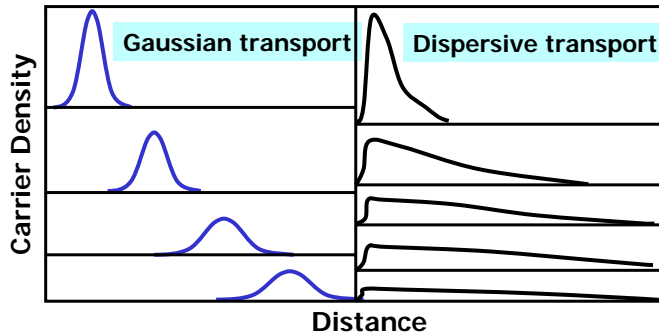
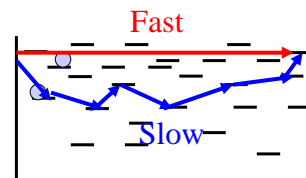
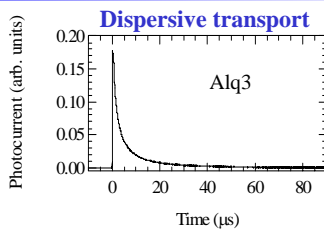
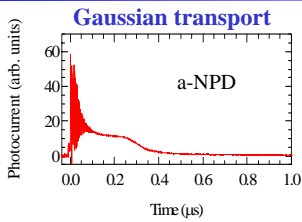


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# Transport of charge carriers in organic materials

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Ref.) Harvey Scher, Michael F. Shlesinger and John T. Bendler, Physics today, Jan. p.26 (1991)



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(1) Poole-Frenkel Model

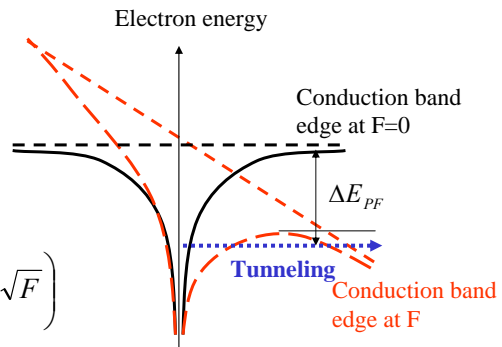
$$\mu(F, T) = \mu_{PF} \exp\left(-\frac{\Delta E - \beta_{PF} \sqrt{F}}{k_B T}\right) \quad \beta_{PF} = \sqrt{\frac{q^3}{\pi \epsilon \epsilon_0}}$$

Carrier mobility shows:

- (i) field-independent activated mobility at low fields, characterized by an activation energy
- (ii) field-dependent mobility of the stretched exponential form  $\exp(\gamma E^{1/2})$  at high fields
- (iii) change of sign of the coefficient  $\gamma$  above a certain emperature.

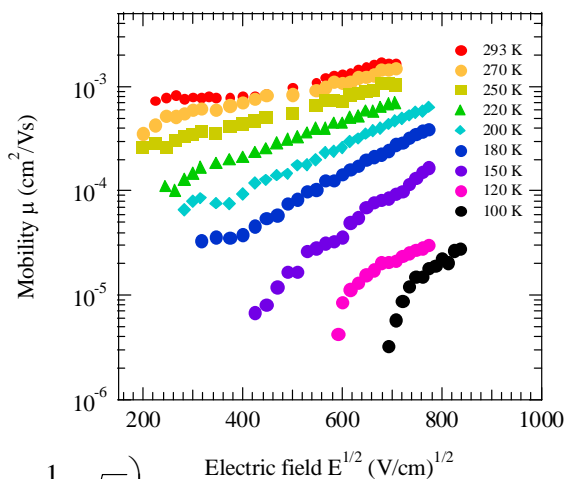
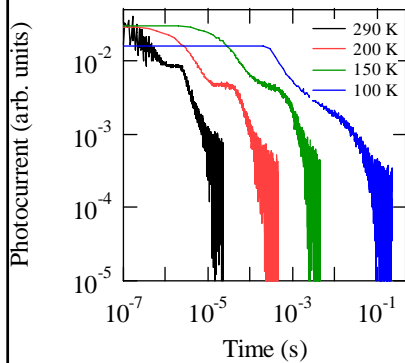
$$\mu(E, T) = \mu_{PF} \exp\left(-\frac{\Delta E}{kT} + \beta_{PF} \left(\frac{1}{kT} - \frac{1}{kT_o}\right) \sqrt{F}\right)$$

W. D. Gill, J. Appl. Phys. **43**, 5033 (1972).



Poole-Frenkel effect

P.W.M. Blom, M.C.J.M. Vissenberg / Materials Science and Engineering 27 (2000) 53-94



$$\mu(E, T) = \mu_{PF} \exp\left(-\frac{\Delta E}{kT} + \beta_{PF} \left(\frac{1}{kT} - \frac{1}{kT_o}\right) \sqrt{F}\right)$$

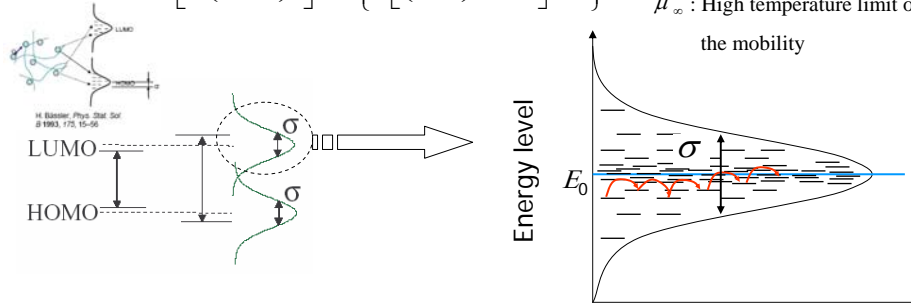


(2) Bassler's gaussian disorder model

- The energy of each site is distributed in accordance with the Gaussian distribution
- Energies of adjacent sites uncorrelated
- Motion between sites is Markovian (no phase memory)

$$\mu(F, T) = \mu_{\infty} \exp\left[-\left(\frac{2\sigma}{3k_B T}\right)^2\right] \exp\left\{C\left[\left(\frac{\sigma}{k_B T}\right)^2 - \Sigma^2\right]\sqrt{F}\right\}$$

$\sigma$  : Energetic disorder  
 $\Sigma$  : Positional disorder  
 $C$  : specific parameter  
 $\mu_{\infty}$  : High temperature limit of the mobility

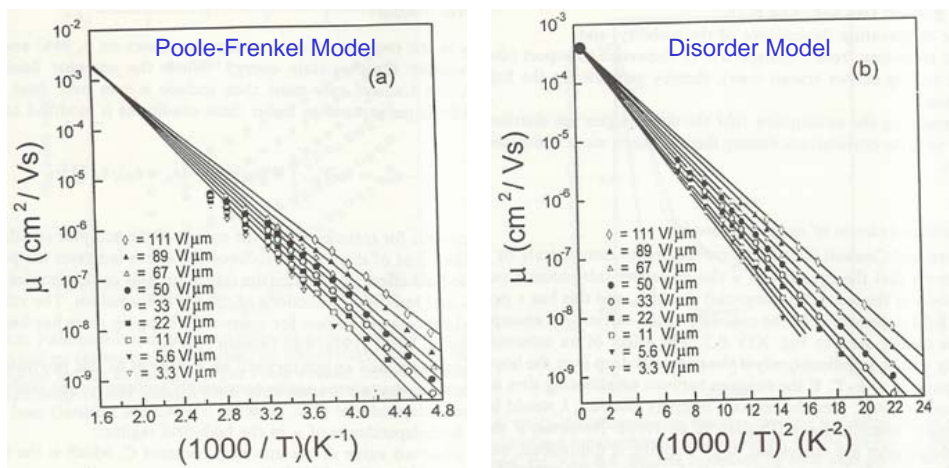


H. Bässler, Phys. Status Solidi B **175**, 15 (1993).

Density of state



Mobility of DEH in polycarbonate



M. Pope and C. E. Swenberg. Electronic Processes in Organic Crystals, (Oxford, New York, 1999), p. 977



# Temperature dependence of the hole mobility of PPVs

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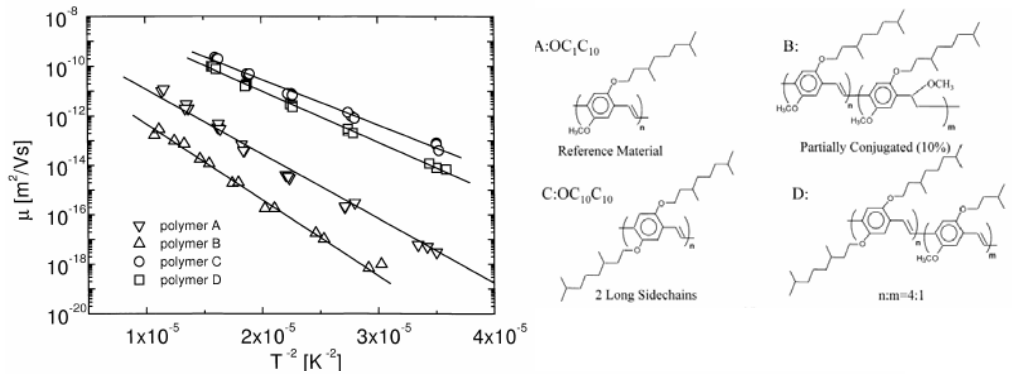


Table 1  
Parameters  $\mu_\infty$ ,  $\sigma$  (energetic disorder bandwidth) and  $a$  (site-spacing) describing the temperature dependence of the zero-field mobility  $\mu_0$  and field activation factor  $\gamma$  for the different polymers studied

Sample	$\mu_\infty$ ( $\text{m}^2/\text{V s}$ )	$\sigma$ (meV)	$a$ (nm)
A	$5.1 \times 10^{-9}$	112	1.2
B	$4.0 \times 10^{-10}$	121	1.7
C	$1.6 \times 10^{-7}$	93	1.1
D	$1.5 \times 10^{-7}$	99	1.2

P.W.M. Blom, M.C.J.M. Vissenberg, Materials Science and Engineering **27**, 53-94 (2000)



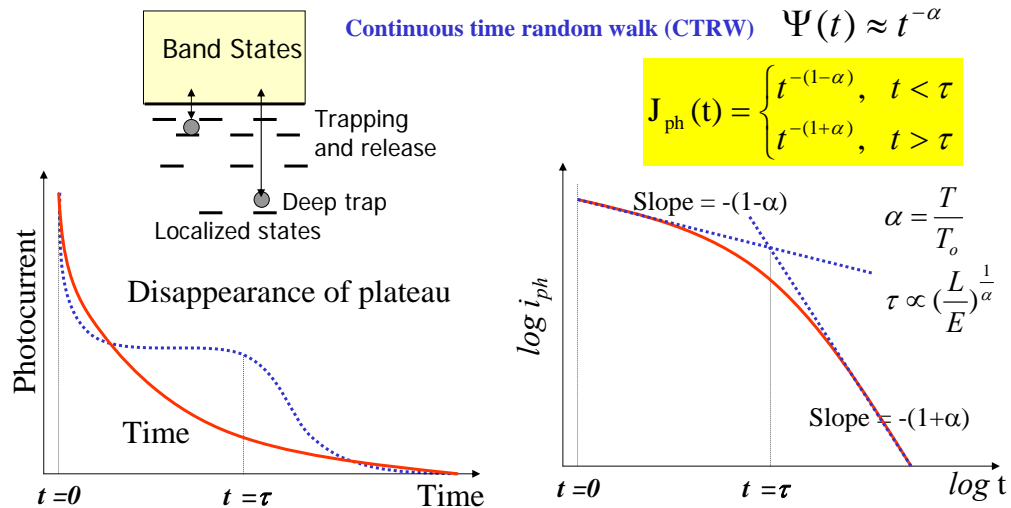
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# Carrier Transport Models

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## (3) Scher-Montroll dispersive transport model



Scher and Montroll, Phys. Rev. B **12**, 2455 (1975)

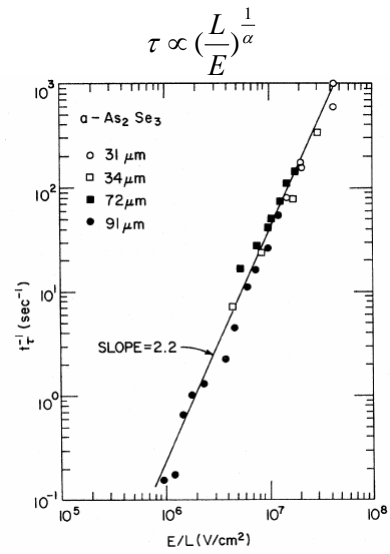
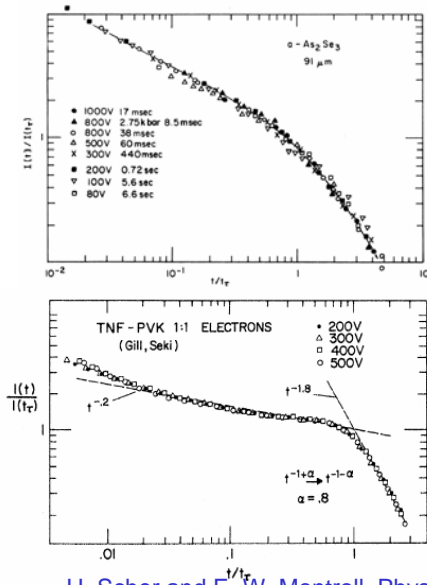


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# Scher-Montroll model of dispersive transport

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H. Scher and E. W. Montroll, Phys. Rev. B 12, 2455 (1975)

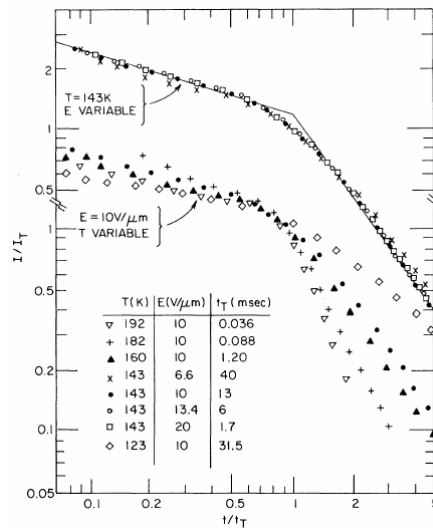
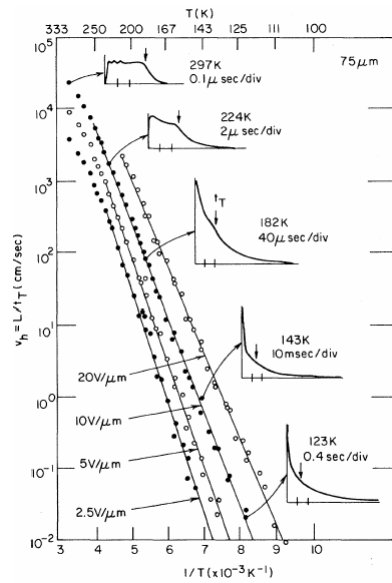


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# Dispersive Transport in α-Selenium

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G. Pfister, Phys. Rev. Lett. 36, 271 (1976)

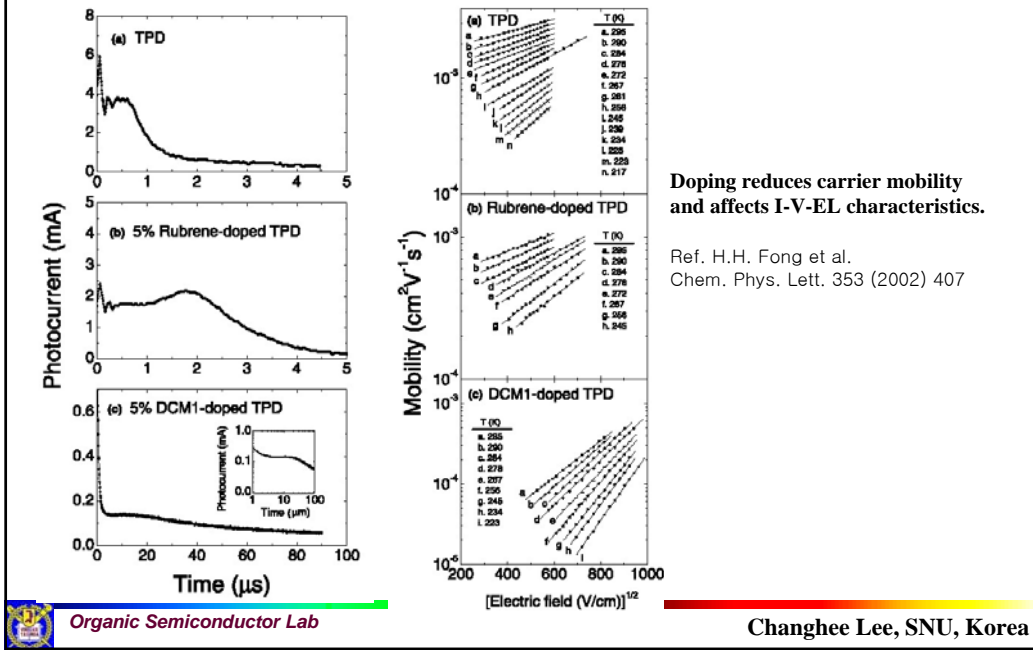


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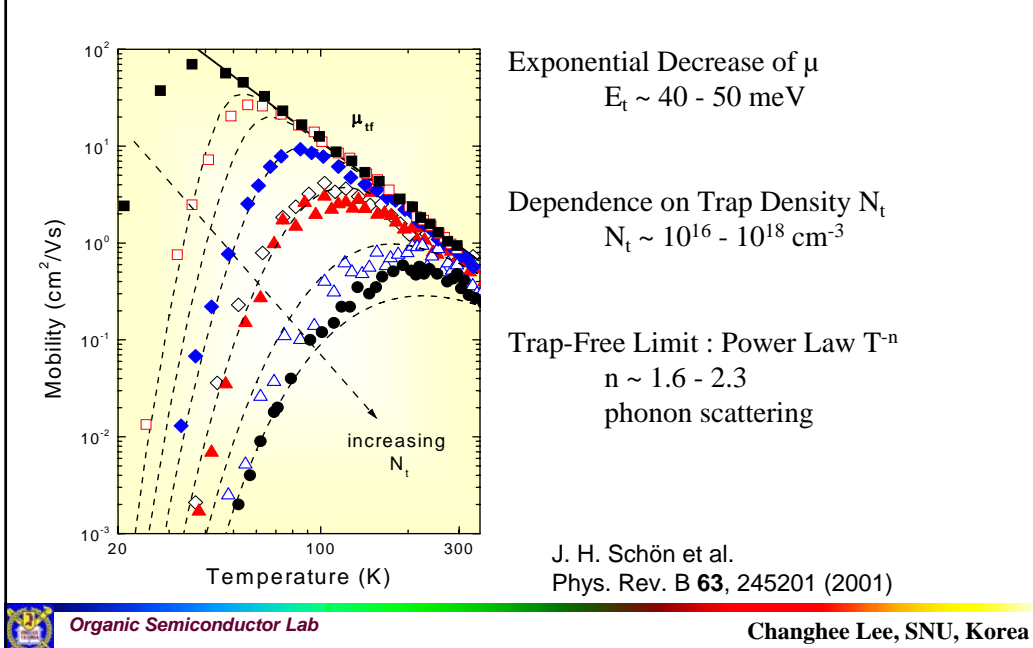
# Mobility – Doping Relation

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# Influence of traps on the carrier mobility

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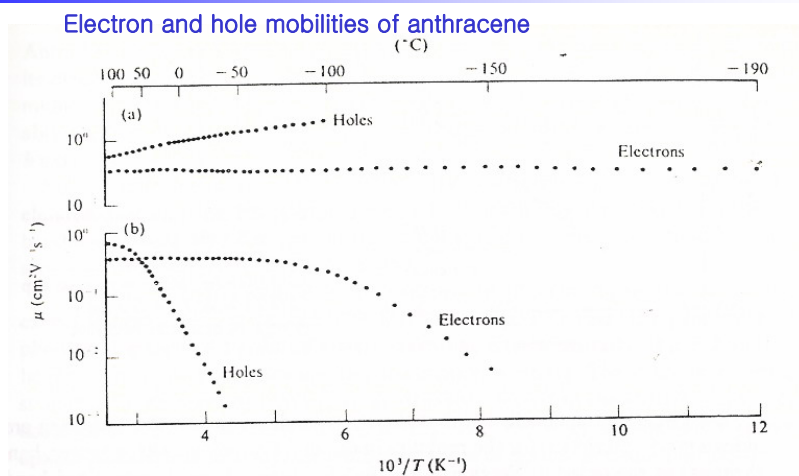


Fig. II.F.14. The influence of  $10^{-7}$  mol/mol tetracene doping on the anthracene  $c'$  charge carrier mobilities. (a) Undoped crystal mobilities; (b) doped crystal mobility. Note the asymmetry between the hole and electron trapping, and the trap depths calculated using Eq. II.F.2.32. (Karl 1980a)

