Transport and noise in organic FETs

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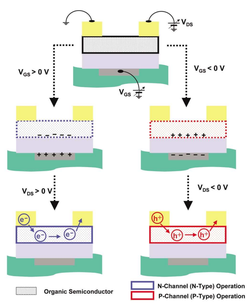
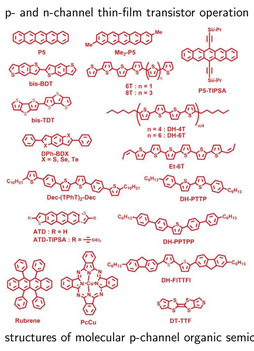
Organic field effect transistors



p- and n-channel thin-film transistor operation



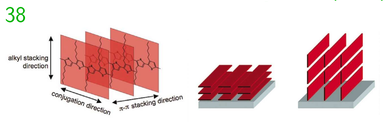
structures of molecular p-channel organic semiconductors

Semiconductor	(cm2/Vs)	Ion/Ioff
Rubrene (air, PMMA)	1.5-20	1.5-20
P5	1.5	10^8
P5 (PVP-CP)	2.9-3.0	10^5
P5 (Al_2O_3)	0.06-0.1	$\sim 10^6$
P5 (SiN_x)	0.2-0.4	$\sim 10^8$
P5 (Ta_2O_5)	0.24	10^4
P5 (Gd_2O_3)	0.1	10^3
P5 TiO2+PαMS	0.8	10^4
P5 (BZT or BST)	0.32-0.60	$\sim 10^5$
P5-precursor	0.01-0.2	$\sim 10^5$
P5-precursor	0.89	$\sim 10^7$
Me_4-P5	0.3	10^3-10^5
P5-TIPSA	0.17	$\sim 10^5$
6T	0.002	
8T	0.33	
DH-6T	0.05	10^3
DH-4T	0.06	10^6
Me_2-6T	0.02	
Et-6T	0.03-0.05	$> 10^5$
Bis-BDT	0.04	
Bis-TDT	0.05	$\sim 10^8$
DPh-BDX	0.01-2.0	$10^3 \rightarrow 10^7$
DH-PTTP	0.09	10^5
DH-PPTPP	0.02	10^4
Dec-$(TPhT)_2$-Dec	0.4	10^5
DH-FITTFI	0.1	10^4-10^5
ADT	0.1	
PcCu	0.02-0.1	$\sim 10^5$
DT-TTF	1.4	$\sim 10^5$
$PcCuTa_2O_5$	0.01	$\sim 10^4$
Bis-BDX	0.17-2.0	10^6-10^7

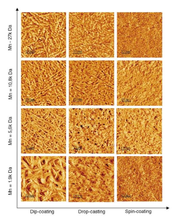
OFET performance of molecular p-channel semiconductors
Antonio Facchetti, materialstoday 10,3 (2007) 28

Stacking

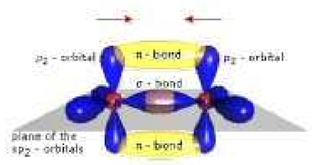
Alberto Salleo, materialstoday 10,3 (2007) 38



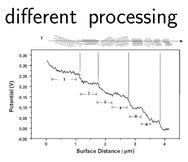
(a) Crystallite structure in polythiophenes. The conjugation direction and the p-p stacking direction are fast charge transport directions. (b) Plane-on (left panel) and edge-on (c) (right panel) texture of polymeric crystallites.



Tapping-mode AFM phase images obtained from P3HT fractions of different Mw and using different processing techniques



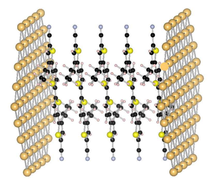
principle of delocalized π electrons



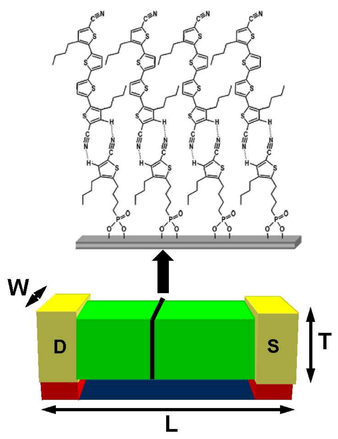
EFM measurement of the potential profile in a conducting polythiophene monolayer deposited between two electrodes

Transport in organic field effect transistors

Parallel stacking of thiophene molecules between 2 Au contacts



$W = 1000\mu m$, $T = 20$nm and $L = 10\mu m$



K. Haubner, et al., phys. stat. sol. (a) 205 (2008) 430

Tight binding model for HOMO, LUMO transport

Hamiltonian

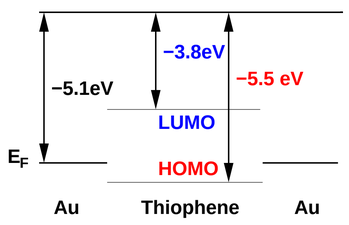
$$H = \sum_{i=-\infty}^{\infty} \left(|i\rangle\, v_i\, \langle i| + |i+1\rangle\, t_{i+1}\, \langle i| + |i-1\rangle\, t_i\, \langle i| \right)$$

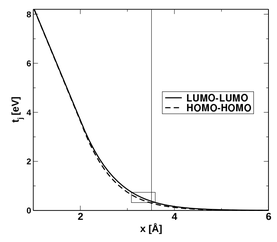
left leads: $j \leq 0$
right leads: $j \geq N+1$

fragment orbital approach with self-consistent charge density-functional based tight-binding (SCC-DFTB) method (Elstner1998,Porezag1995,Seifert1996)

$$T_{ij} = \left\langle \phi_i | \hat{H}_{KS} | \phi_j \right\rangle$$

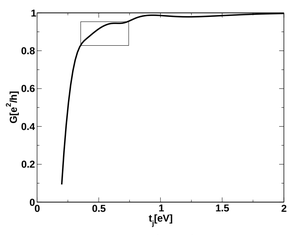
whith Kohn-Sham Hamiltonian H_{KS}



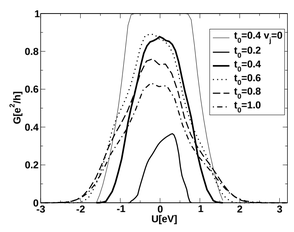


Currents with surface Green functions

Conductance $G = \frac{e^2}{U} \int \frac{dz}{2\pi\hbar} T_{N+1,0} \left(f_r - f_l \right)$

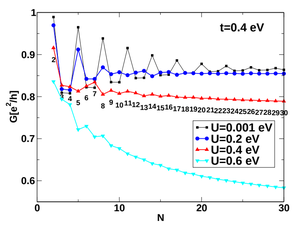


20 Thiophene molecules

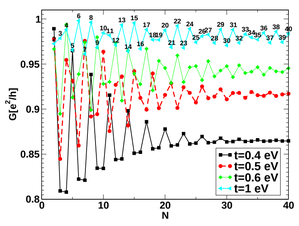


versus applied voltage bias for different hopping parameters from lead to thiophene, $v_0 = 0$, $v_j = -0.4$, reference curve $v_j = 0$

Current oscillation



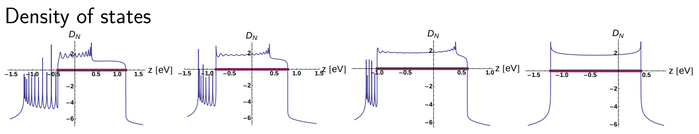
conductance versus number of thiophene molecules between Au contacts for different voltages



number of molecules between Au leads in linear response regime

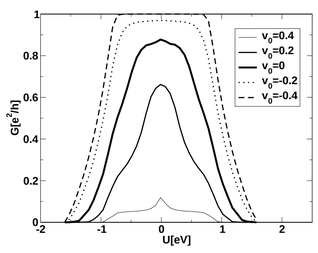
Lead design, e.g by barrier

Density of states

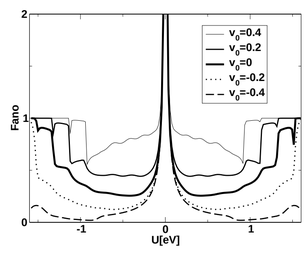


$v_0 = 0.4eV$ $v_0 = 0eV$ $v_0 = -0.2eV$ $v_0 = -0.4eV$

Conductance



Fano factor $\frac{\overline{\Delta J \Delta J}}{eJ}$



Thermoelectric properties

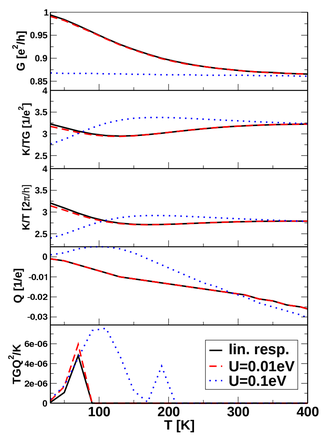
Temperature difference
at right: $T_r = T + \Delta T/2$ and left lead: $T_r = T - \Delta T/2$

$$\text{particle current} \quad J = L^{11} V + L^{12} \Delta T$$
$$\text{heat current} \quad J_q = L^{21} V + L^{22} \Delta T$$

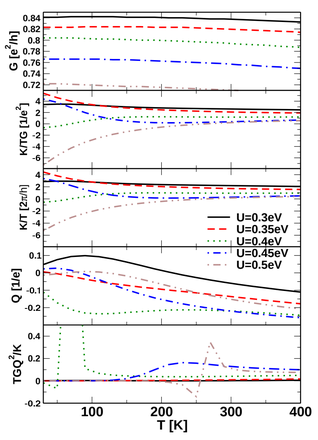
- conductance, $J = GV$: $G = L^{11}$
- thermoelectric power, $V = -Q\Delta T$ with $J = 0$: $Q = \frac{L^{12}}{L^{11}}$
- thermoelectric conductance, $J_q = K\Delta T$ with $J = 0$: $K = L^{22} - \frac{L^{21}L^{12}}{L^{11}}$
- figure of merit or ZT factor: $ZT = \frac{TQ^2G}{K} = \frac{T(L^{12})^2}{L^{11}L^{22} - L^{21}L^{12}}$

Conductance, heat conductance, thermopower, figure of merit

near the linear response



beyond linear response



Summary

- Hopping transport in organic FET conveniently described by surface Greenfunctions
- Current staggering in dependence of number of molecules
- Transport properties can be engineered by shaping leads
- Thermoelectric properties possible to design by geometry, barrier height, hopping parameter and temperature regime
- Nonlinear voltage bias leads to large resonances in figure of merit at special temperatures

Thanks to collaboration (2 recent papers):

- New J. Phys. **10** (2008) 103014-1-8: *Current without bias and diode effect in shuttling transport of nanoshafts*, K. Morawetz ,S. Gemming, R. Luschtinetz, L. M. Eng, G. Seifert, A. Kenfack
- Phys. Rev. B **79** (2009) 085405-1-12: *Transport and noise in organic field effect devices*, K. Morawetz, S. Gemming, R. Luschtinetz, T. Kunze, P. Lipavský, L. M. Eng, G. Seifert, P. Milde

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