Current without bias in shuttling of nanoshafts

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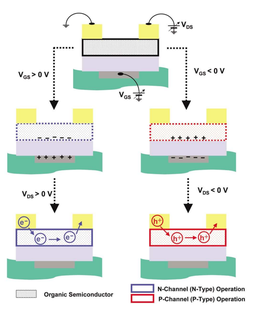
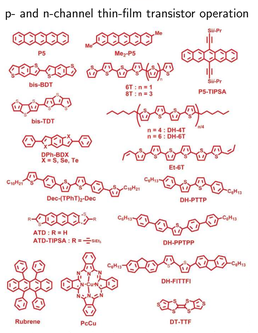
Organic field effect transistors



p- and n-channel thin-film transistor operation



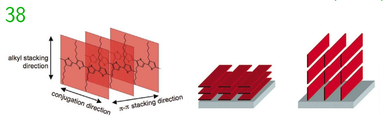
structures of molecular p-channel organic semiconductors

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

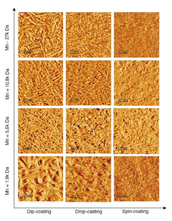
OFET performance of molecular p-channel semiconductors
Antonio Facchetti, materialstoday 10,3 (2007) 28

Stacking

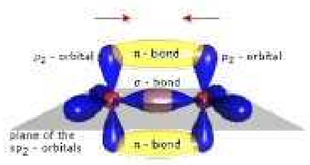
Alberto Salleo, materialstoday 10,3 (2007) 38



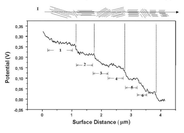
(a) Crystallite structure in polythiophenes. The conjugation direction and the p-p stacking direction are fast charge transport directions. (b) Plane-on (left panel) and edge-on (c) (right panel) texture of polymeric crystallites.



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



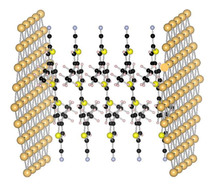
principle of delocalized π electrons

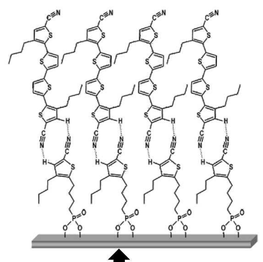


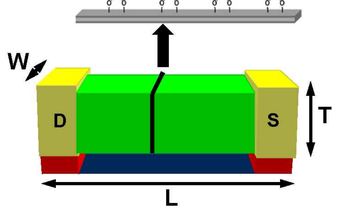
EFM measurement of the potential profile in a conducting polythiophene monolayer deposited between two electrodes

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

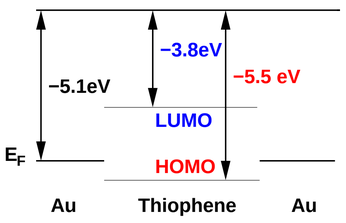
Funding via the Deutsche Forschungsgemeinschaft (SPP 1155) and the DFG-BMBF Programme GEOTECHNOLOGIEN is gratefully acknowledged.

Tight binding model for HOMO, LUMO transport

Hamiltonian

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

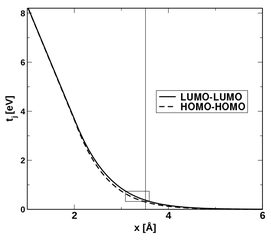
left leads: $j \leq 0$
right leads: $j \geq N+1$



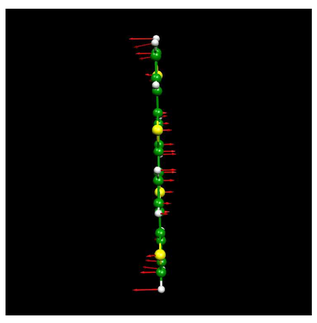
fragment orbital approach with self-consistent charge density-functional based tight-binding (SCC-DFTB) method (Elstner1998,Porezag1995,Seifert1996)

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

whith Kohn-Sham Hamiltonian H_{KS}



Diode effect in shuttling transport



Parameter from DFT calculations:

k=1 N/m, m=5.49x10^{-22}g, ω=1.35/ps, l_0=0.1nm
[E]=$m\omega^2 l_0/q$=6.2x10^8V/m,
[J]=$q\omega$=21.6mA

Model

- consider N nanoshafts of length L parallel oriented in y-direction perpendicular to substrate
- couple elastically by top ends and bend in x direction applying tangential force F

$$x(z) = \frac{Fz^2}{2\mathcal{E}I}\left(L - \frac{z}{3}\right) = \frac{3}{2}x(L)\left(\frac{z}{L}\right)^2\left(1 - \frac{z}{3L}\right)$$

where $\mathcal{E}$ Young modulus and $I = \int z^2 dA$ area moment of inertia
- maximal displacement on the top ends $z = L$ is $x \equiv x(l) = FL^3/3\mathcal{E}I$ from which the spring constant $k = F/x = 3\mathcal{E}I/L^3$ is given
- nanoshafts are located between two oppositely charged plates
- each nanoshaft can carry $q_i < 0$ describing charge in LUMO or $q_i > 0$ for transport of holes in HOMO or none which can be exposed to time-dependent external field $E(t)$
- coupled linear chain of top ends obeying

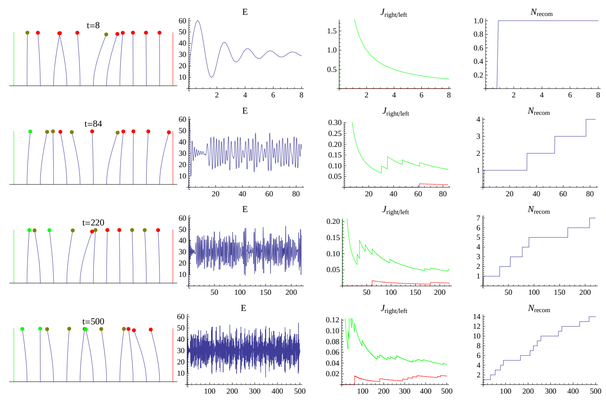
$$\frac{d^2 x_i(t)}{dt^2} = \omega^2[x_{i-1}(t) - 2x_i(t) + x_{i+1}(t)] + a_i(t)$$

with the force per mass $\omega^2 = 3\mathcal{E}I/mL^3$ and accelleration due to external bias $a_i(t) = q_i E(t)/m$
- time in units of $1/\omega$ further
- analytical solution in terms of normalized orthogonal system $\phi_{n\nu} = \sqrt{2/(N+1)}\sin[n\nu\pi/(N+1)]$,

$$x_i(t) = \sum_{n=1}^{N} \phi_{ni}\left[(c_n \cos\omega_n t + d_n \sin\omega_n t) + \int_0^t dt' \frac{\sin\omega_n(t-t')}{\omega_n} \sum_{m=1}^{N} a_m(t')\phi_{nm}\right]$$

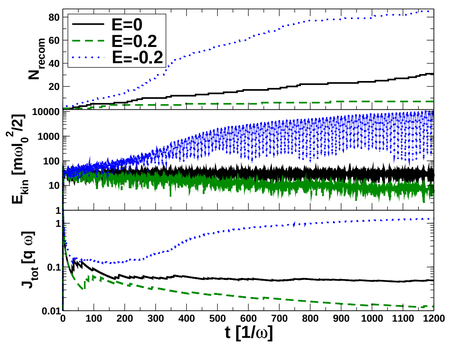
with eigenfrequencies $\omega_n^2 = 2(1 - \cos[n\pi/(N+1)])$
- when two top ends touch each other, charge is moved if one of both tubes had no charge, in case of opposite charges they annihilate counted as recombination which gives rise to light emission
- when such event happens, time evolution according to analytical solution restarts with new initial conditions and new charge distribution, in this way speed of analytical solution together with nonlinear process of recharging

Chain shuttling

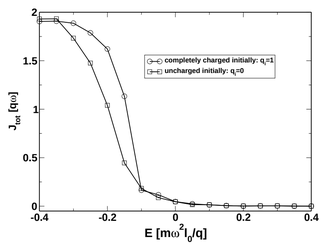


Four snapshots of time evolution (from above to below) of the chain of shuttling nanoshafts (1. row) with positive charge (green) and negative charge (red) or no charge state (grey). The kinetic energy E (2. row), left (green) and right (red) side currents $J_{right/left}$ (3. row) and the number of recombinations N_{recom} (4. row) is given versus time elapsed

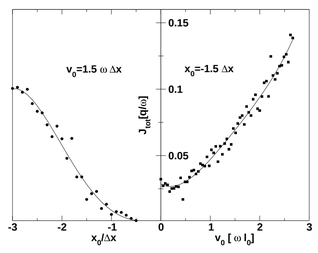
Diode effect



Time evolution for number of recombinations (above), total kinetic energy (middle) and total current (below) for 3 different applied fields



total current versus applied electric field



versus initial displacement (left) and initial velocity (right)

Summary

- Chain of perpendicularly arranged coupled and chargeable nanoshafts show a shuttling transport of charges
- A finite current is established already without external bias only due to the initial asymmetric deformation of the nanoshafts
- For transport between thiophene molecules, besides the hopping also shuttling transport channel is of importance
- Hopping transport in organic FET conveniently described by surface Greenfunctions (see Poster SYOP 4.26)
- 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