Transport through Nanostructures

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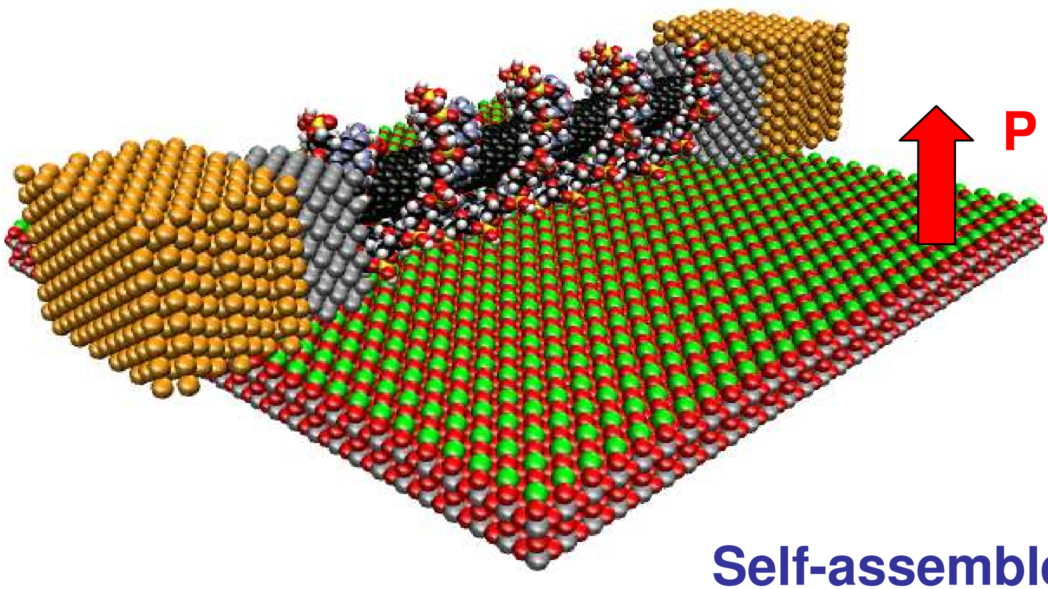
Pf 510119, D-01314 Dresden

Organic field-effect transistor on ferroic substrate

FET-prototype



Self-assembled monolayer gate?

Continuous wire/tube gate?

Switching?

Gate: (7,3)CNT @ polyG-DNA
Contact: Ti/Au electrodes
Field: $BaTiO_3$ surface polarisation

Scale-bridging approaches

L [m] **t [s]**

L [m]	t [s]
10^{0}	10^{0}
10^{-3}	10^{-3}
10^{-6}	10^{-6}
10^{-9}	10^{-9}
10^{-12}	10^{-12}

Scale-Hopping

Parameter-Transfer

Micromechanics
BCF-Phase-field with concentrations

Ising/Heisenberg
Monte-Carlo (MC) with molecules/spins

(Semi-)Empirical Theory
molecular dynamics (MD) with atoms

First-principles Theory
quantum mechanics with electrons

Scale-Coupling

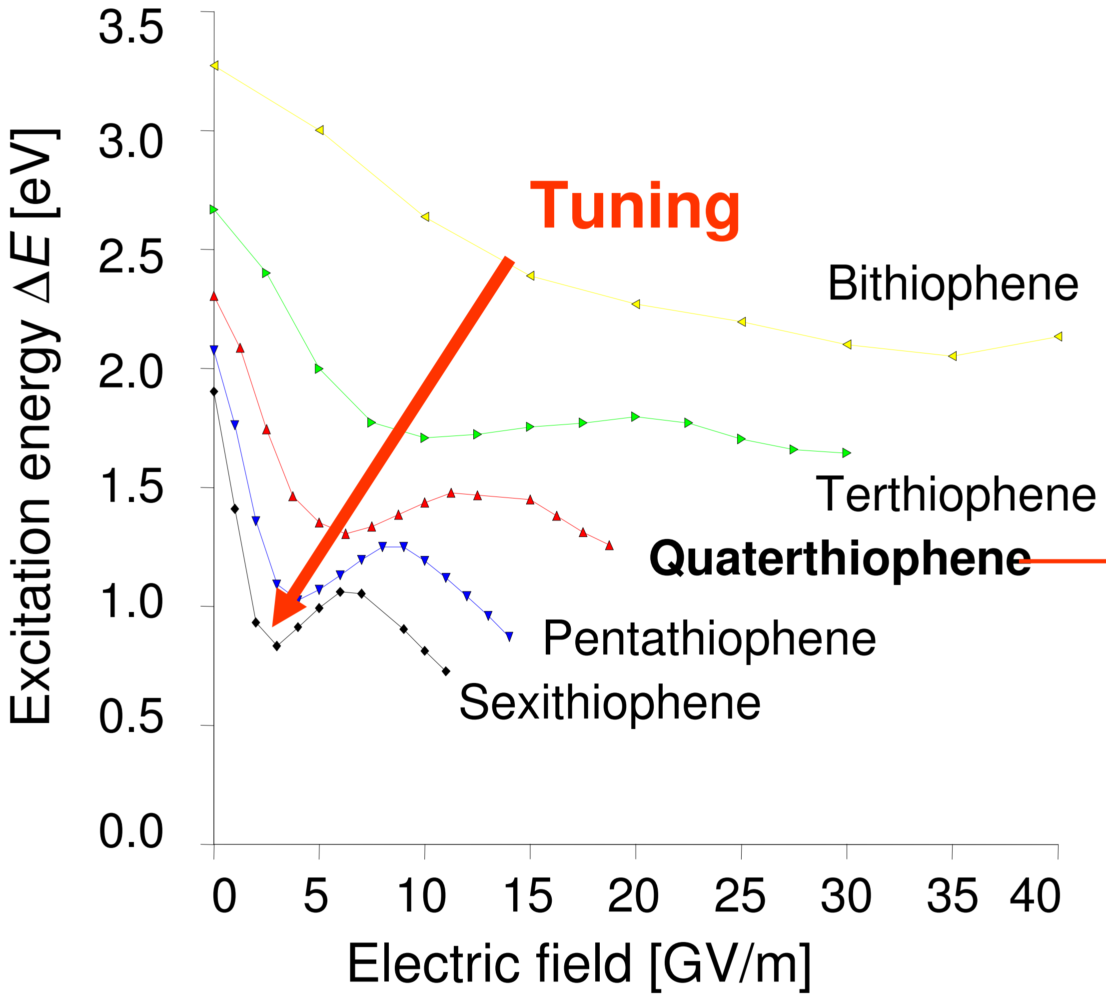
PP/MC
RWTH

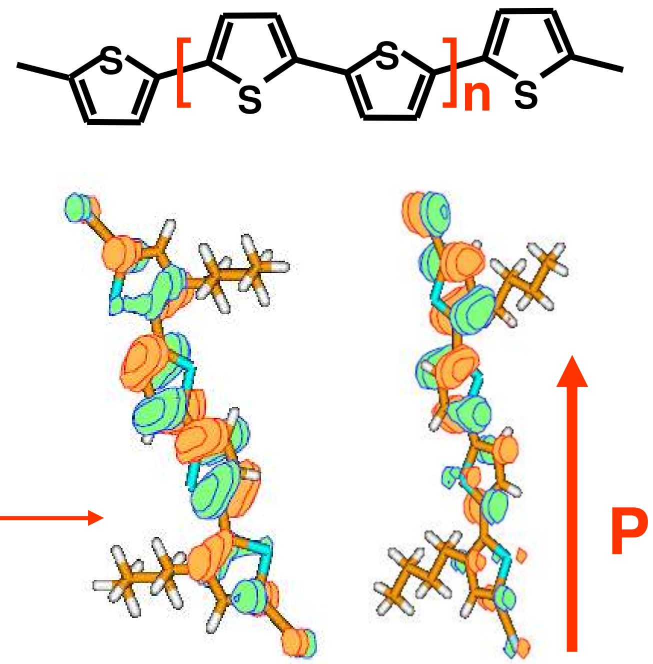
QM/MM
QM/QM‘
TUD

Self-assembled monolayer gate

Thiophenes

Field sensitivity of oligothiophenes





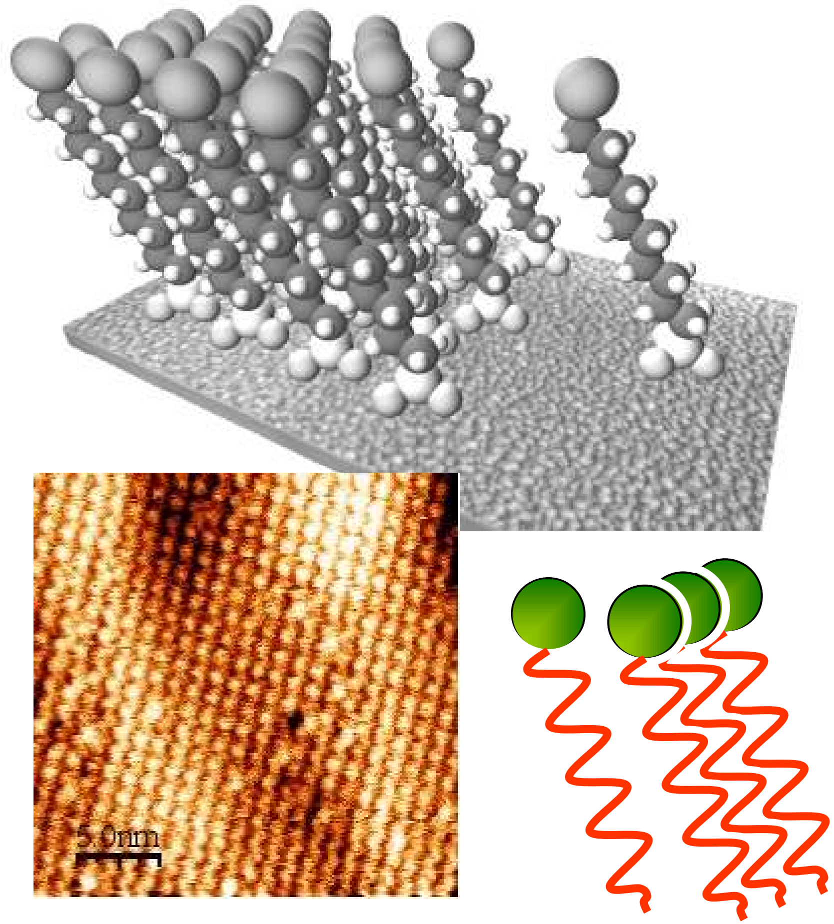
J Computer-Aided Mater Des (2007) 14:211–218
DOI 10.1007/s10820-007-9076-7

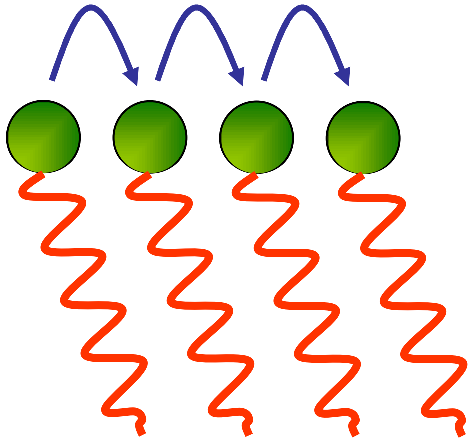
Modelling ferroic functional elements

S. Gemming · R. Luschtinetz · W. Alsheimer
G. Seifert · Ch. Loppacher · L. M. Eng

Transport mechanisms

Self-organized QT layer

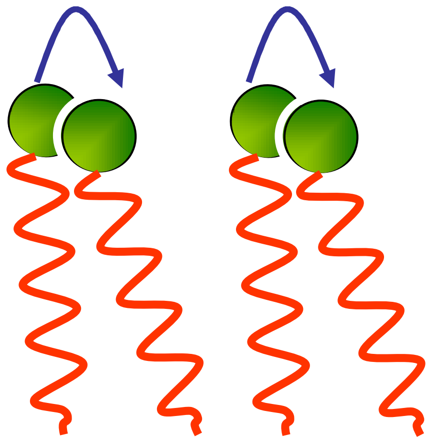




Hopping

classical
master equation

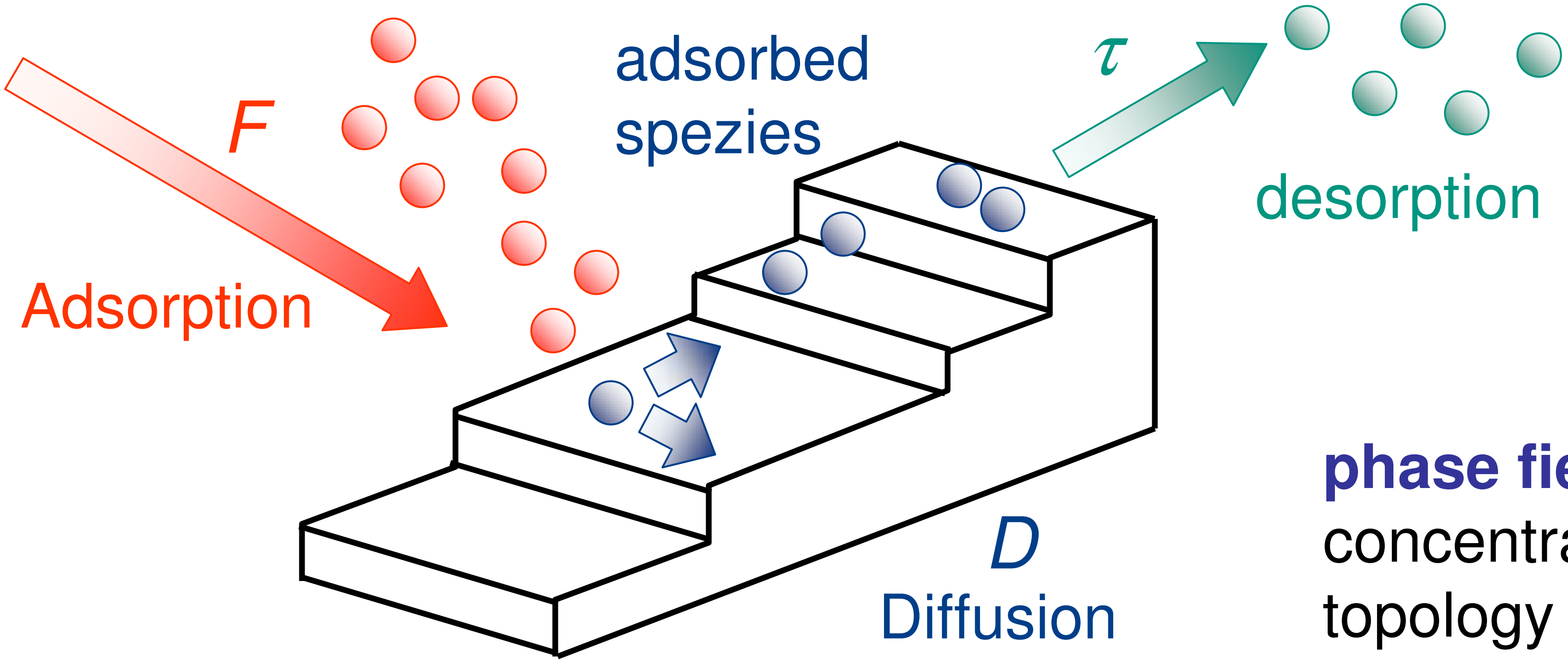
semi-classical
tight-binding



Shuttling

classical
elasto-mechanics

Self-assembly – Burton-Cabrera-Franck



phase field
concentration *n*
topology ψ

DFT-HF/MP2
interactions
molecule-molecule
molecule-surface

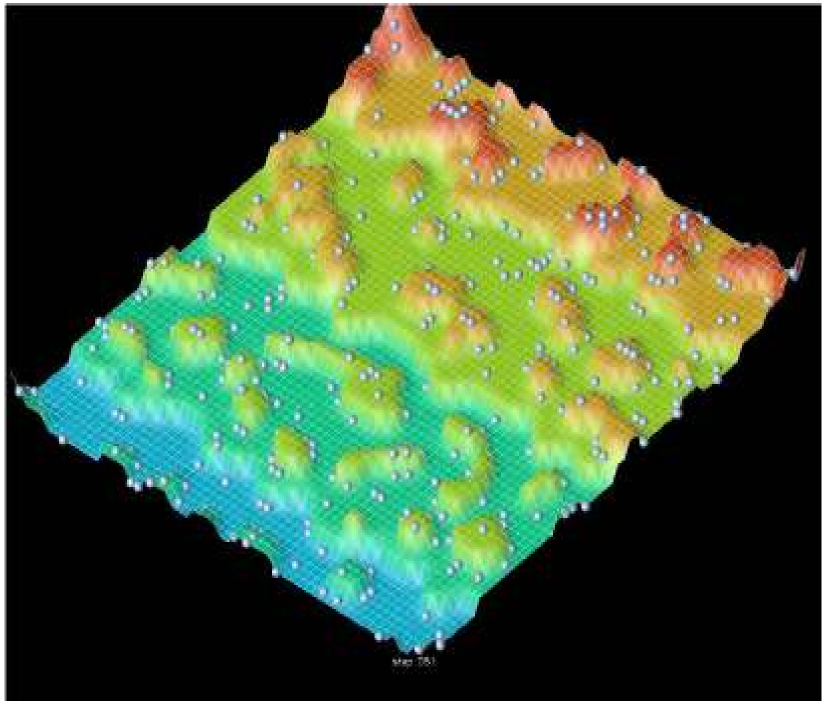
J, H

Metropolis-Monte-Carlo

$\langle D \rangle, \langle \tau \rangle, \langle n \rangle$

Growth modes on structured surfaces

Island – layer-growth



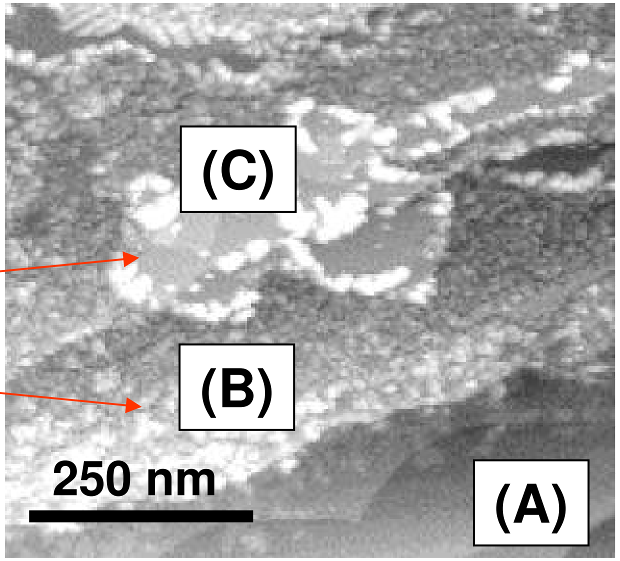
(T = 400 K, D = 3.2 x 10^5 a^2/s,
F = 3 ML/ms, τ = 10^4 s)

Radke, Kundin, Emmerich, Gemming,
Physica D ***238*** *(2009)* 117-125.

PTCDA on KBr|Ag

layer

islands



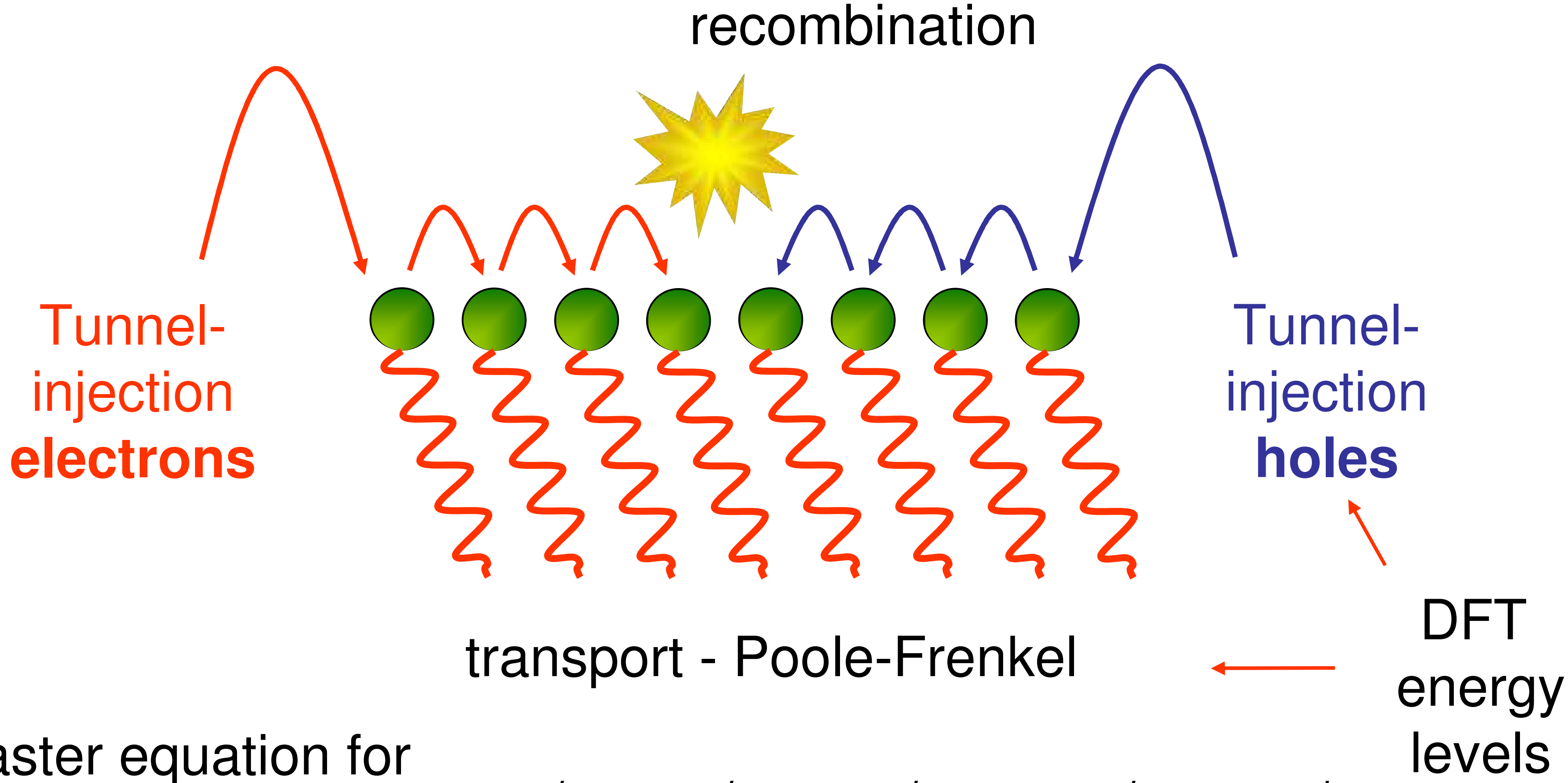
(f_0 = 155.926 kHz, k = 40 N/m,
Δf = 34 Hz, A_0 = 1,7 nm)

Institute of Physics Publishing
Nanotechnology 17 (2006) 1568–1573

Adsorption of PTCDA on a partially KBr covered Ag(111) substrate

Ch Loppacher[1,4], U Zerweck[1], L M Eng[1], S Gemming[2], G Seifert[2], C Olbrich[3], K Morawetz[3] and M Schreiber[3]

Classical hopping

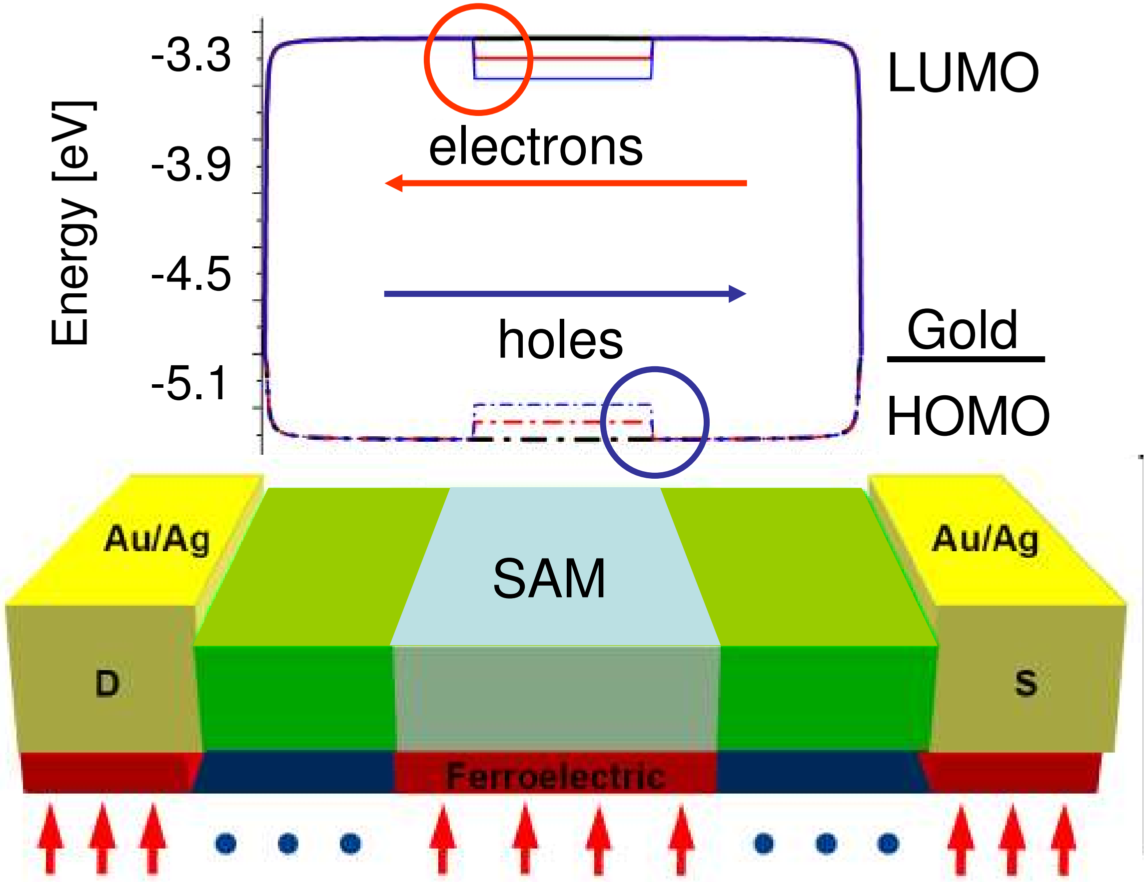


Master equation for carrier densities at each site i

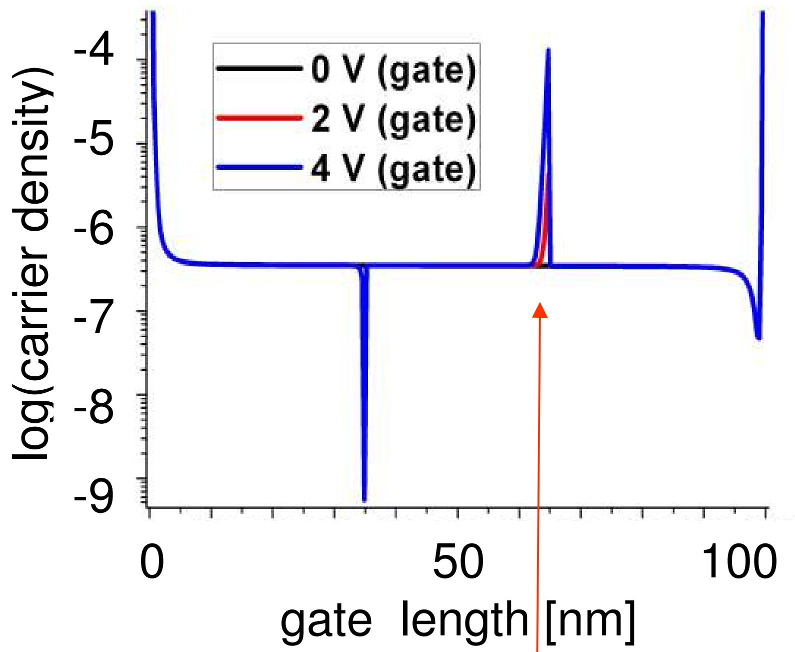
$$n^i_{new} = n^i_{old} + \Delta n^i_{trans} + \Delta n^i_{tunn} - \Delta n^i_{rec}$$

Hopping transport

Ferroelectric domain: Δ*E*



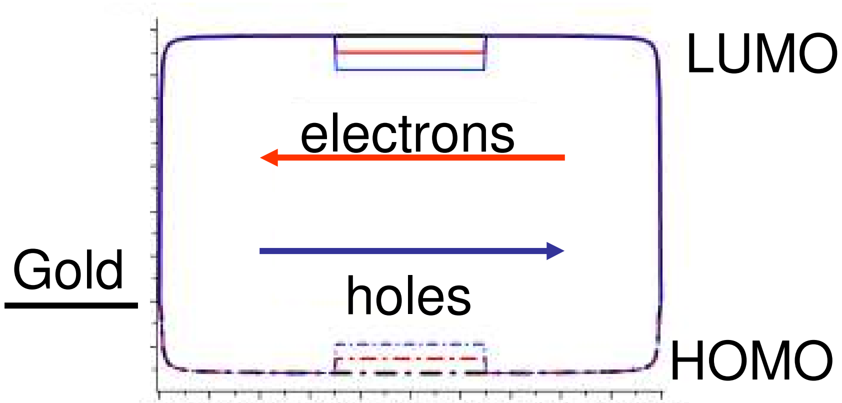
Majority carrier: holes



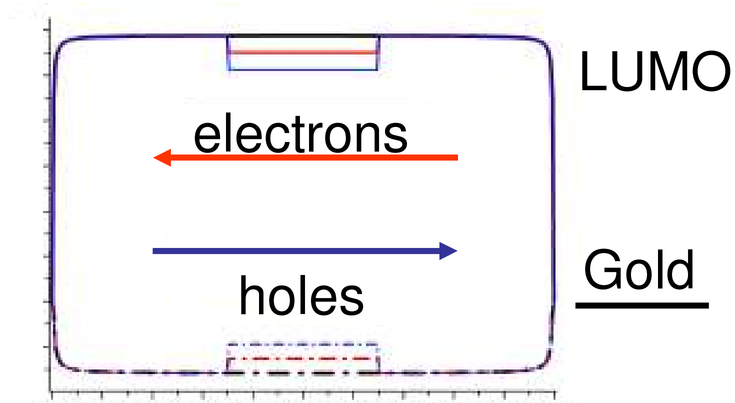
accumulation
increased mobility

Hopping transport - Modifications

Contact metal



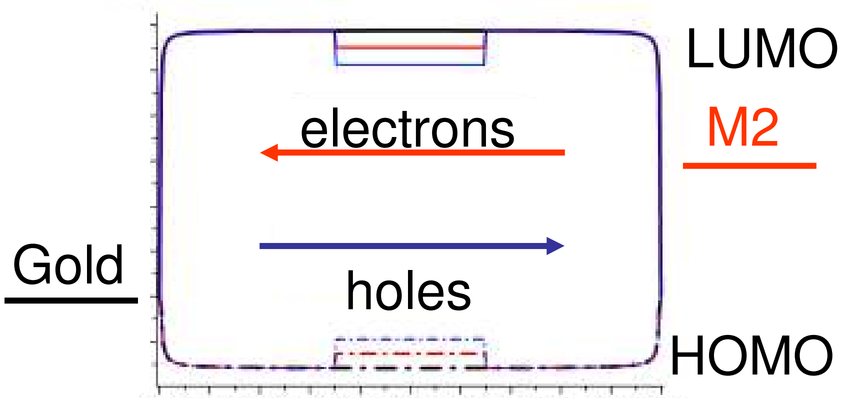
Anchoring group



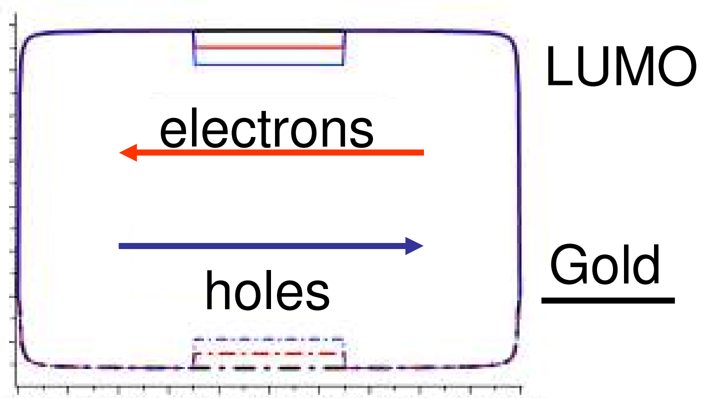
Structure of Matter

Hopping transport - Modifications

Contact metal



Anchoring group



two-level transport

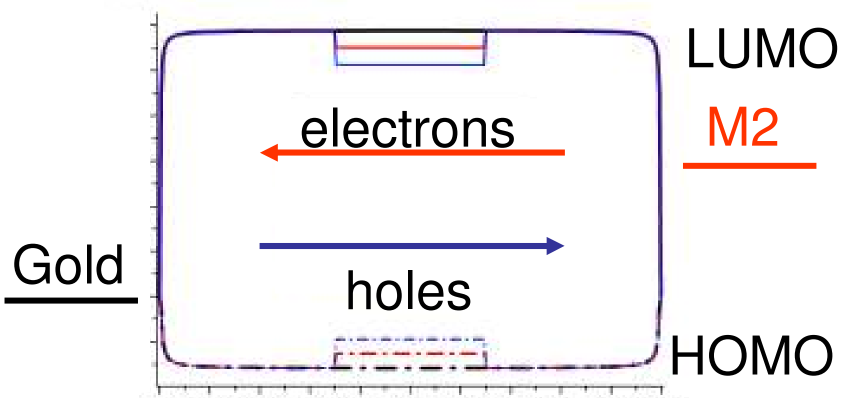
diode effect

Nikolai B Zhitenev[1,3], Artur Erbe[1,4], Zhenan Bao[1,5], Weirong Jiang[1,2] and Eric Garfunkel[2]

Nanotechnology **16** (2005) 495–500

Hopping transport - Modifications

Contact metal



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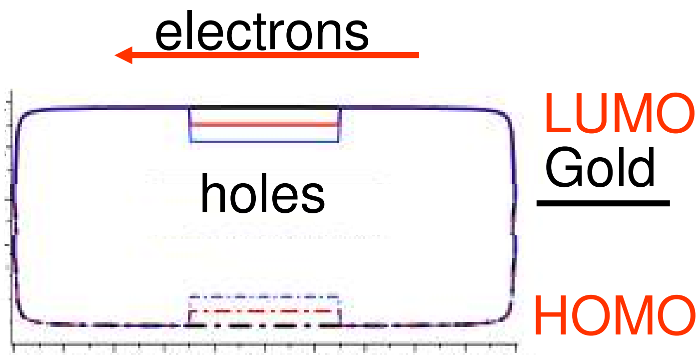
Anchoring group



single-level transport

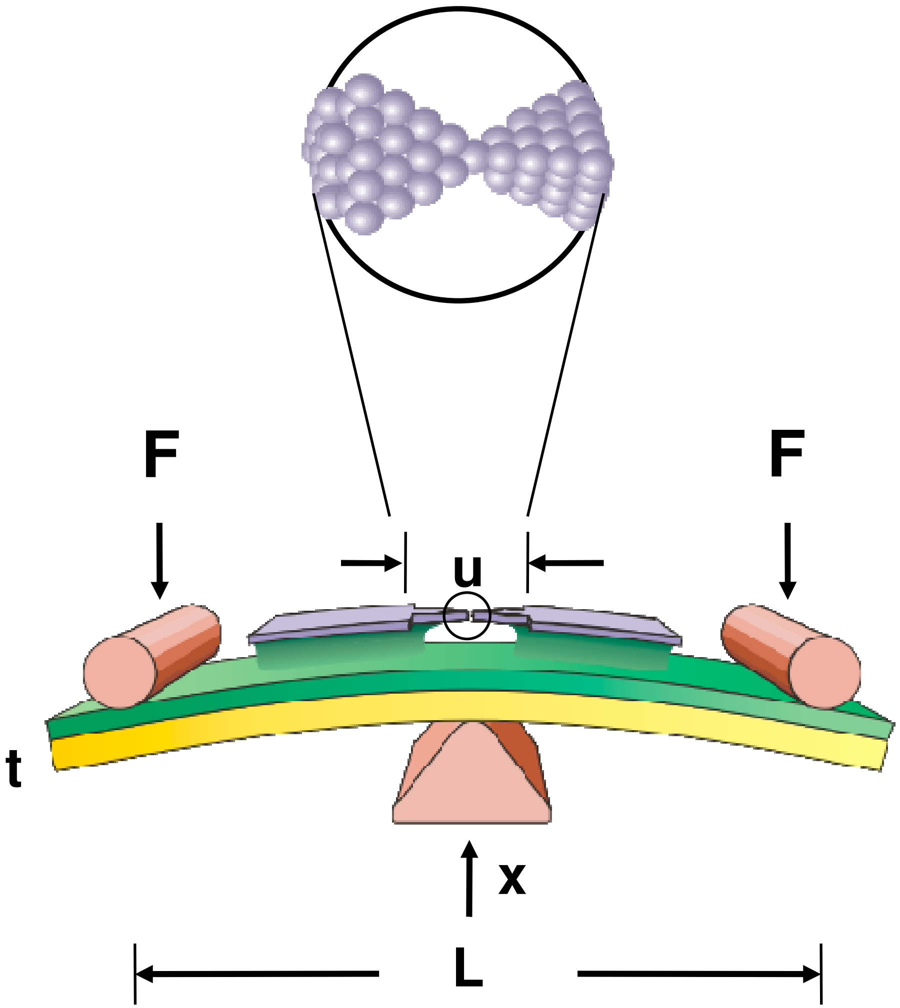
HOMO: SH, LUMO: CN

majority carrier h^+ / e^-

A. Erbe et al.

small 2010, 6, No. 14, 1529–1535

Mechanically controlled break junctions



bending by δx

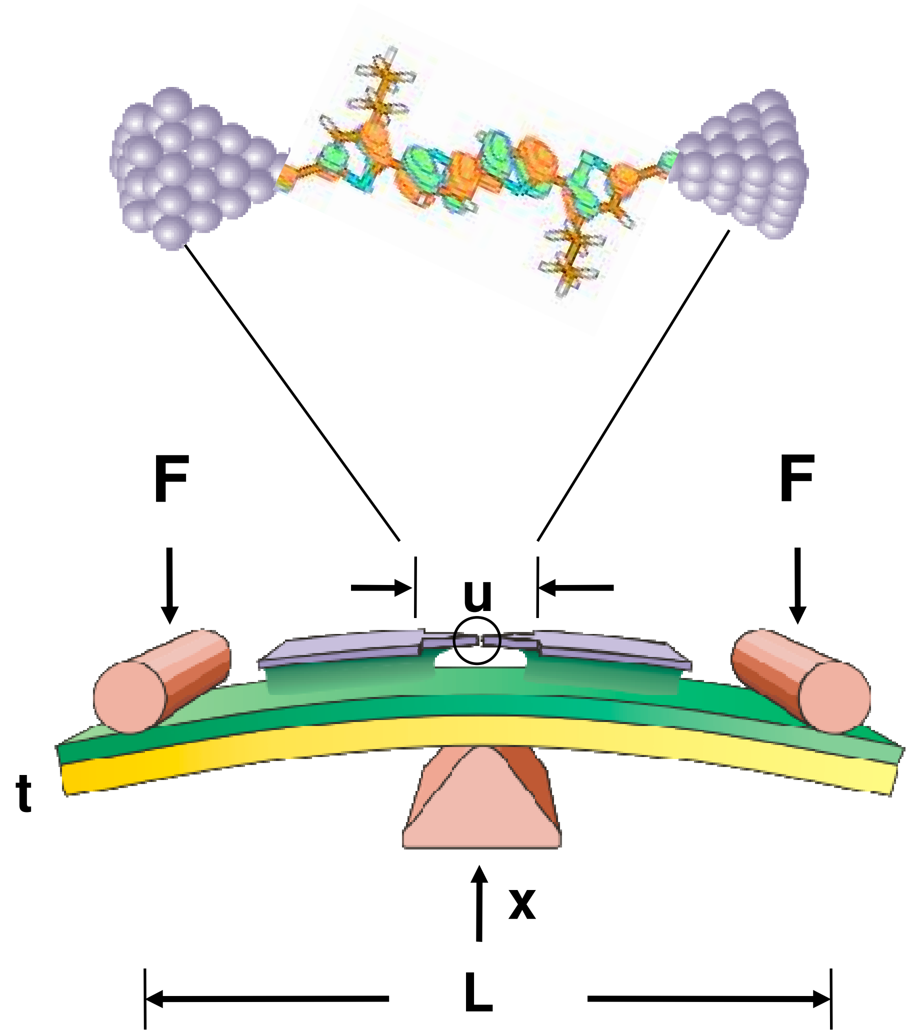
lateral stretching: $\delta u = r\,\delta x$

$(r \sim 10^4 - 10^5)$

= atomic resolution

with “simple” mechanics

Mechanically controlled break junctions



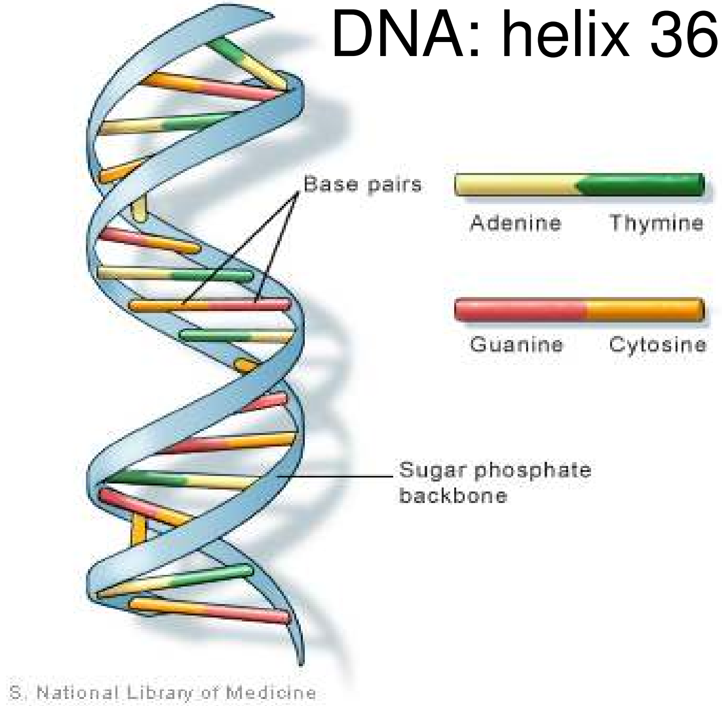
bending by δx

lateral stretching: $\delta u = r\,\delta x$
$(r \sim 10^4 - 10^5)$
= atomic resolution
with "simple" mechanics

insert molecule
& measure transport

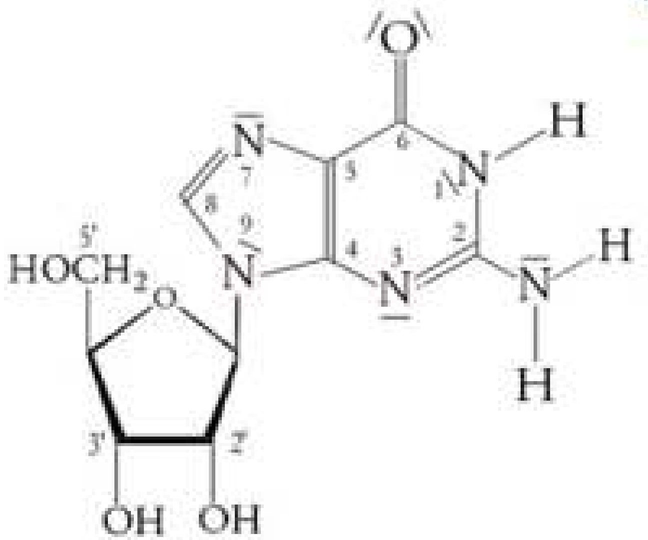
Transport through DNA quadruplexes

DNA: helix 36°



nucleosides:

G = guanosine



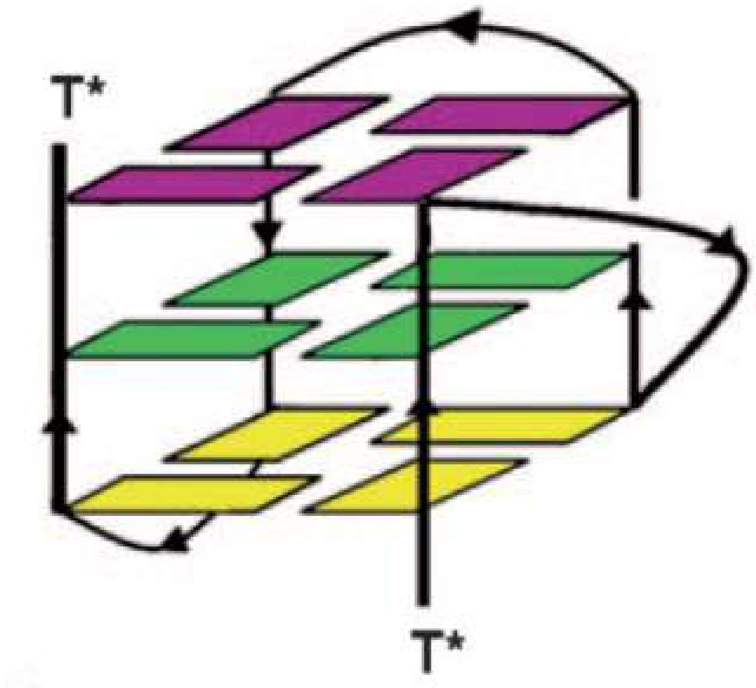
Angewandte Chemie International Edition

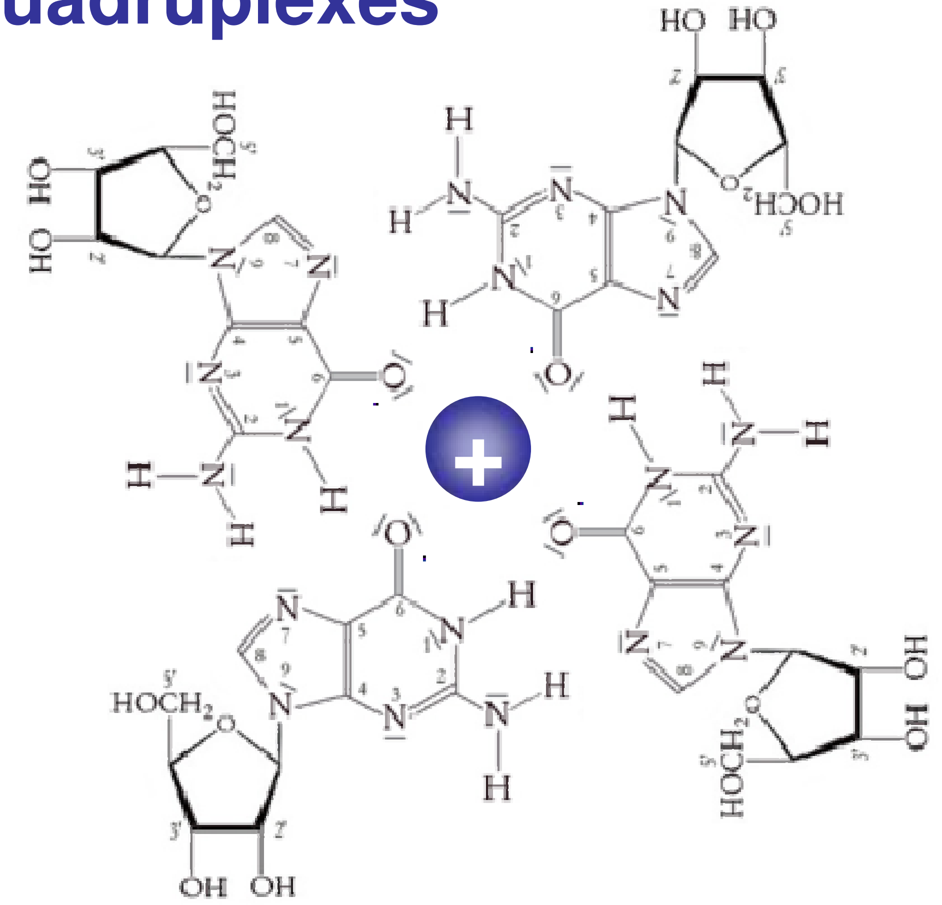
Direct Measurement of Electrical Transport Through G-Quadruplex DNA with Mechanically Controllable Break Junction Electrodes**

*Shou-Peng Liu, Samuel H. Weisbrod, Zhuo Tang, Andreas Marx, Elke Scheer, and Artur Erbe**

Transport through DNA quadruplexes

G quadruplex





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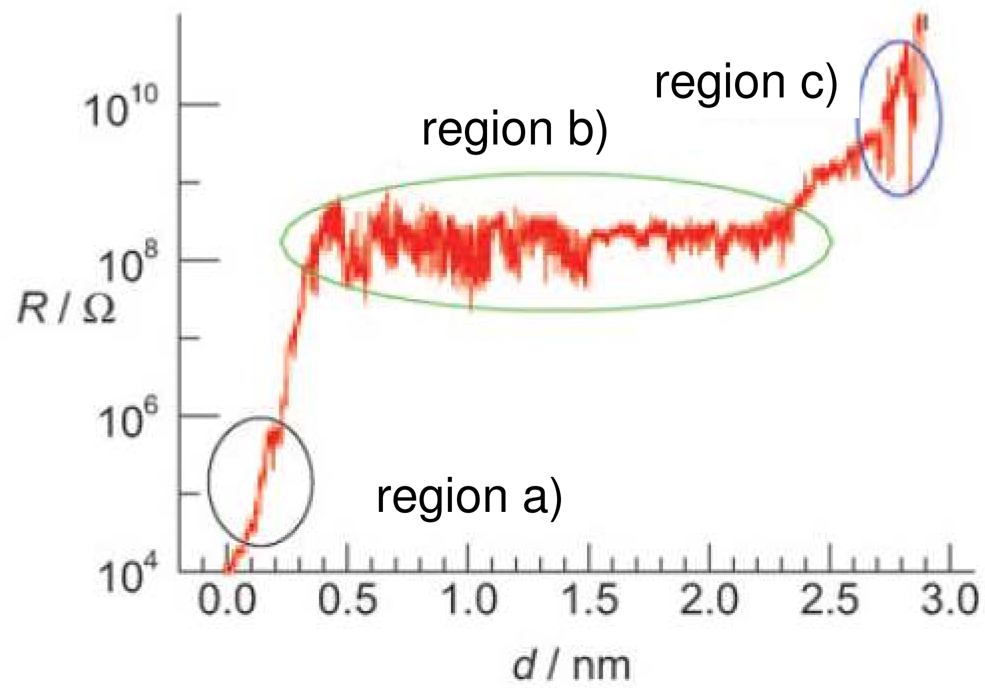
Transport through DNA quadruplexes

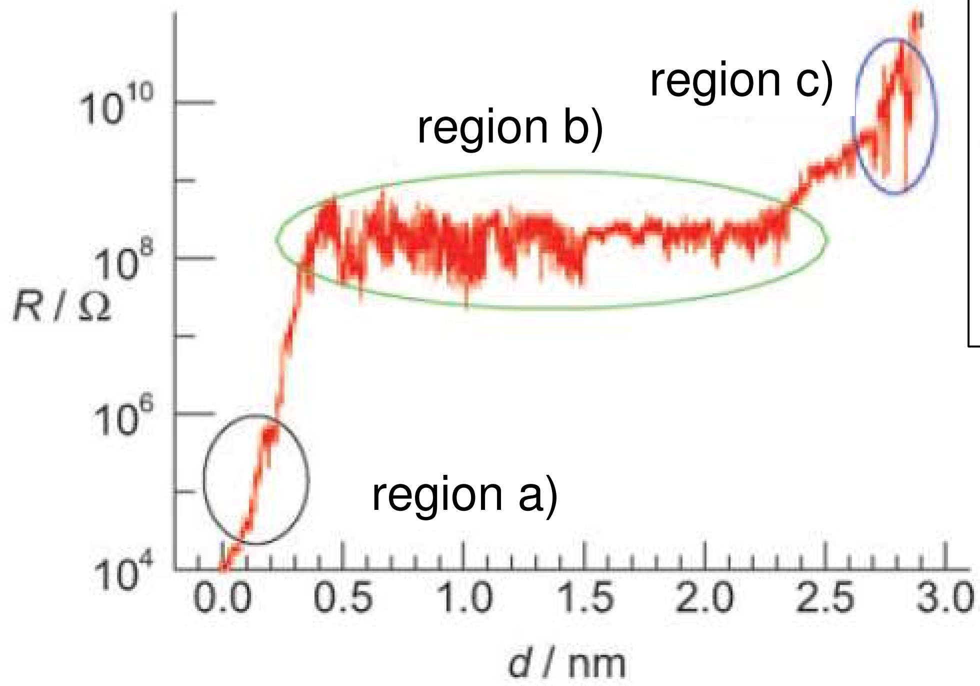
Resistance-distance dependence

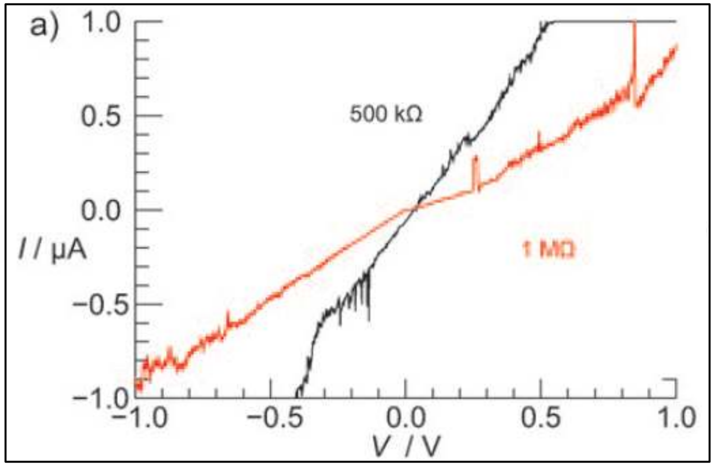


Three stage behaviour?

Transport through DNA quadruplexes

Resistance-distance dependence

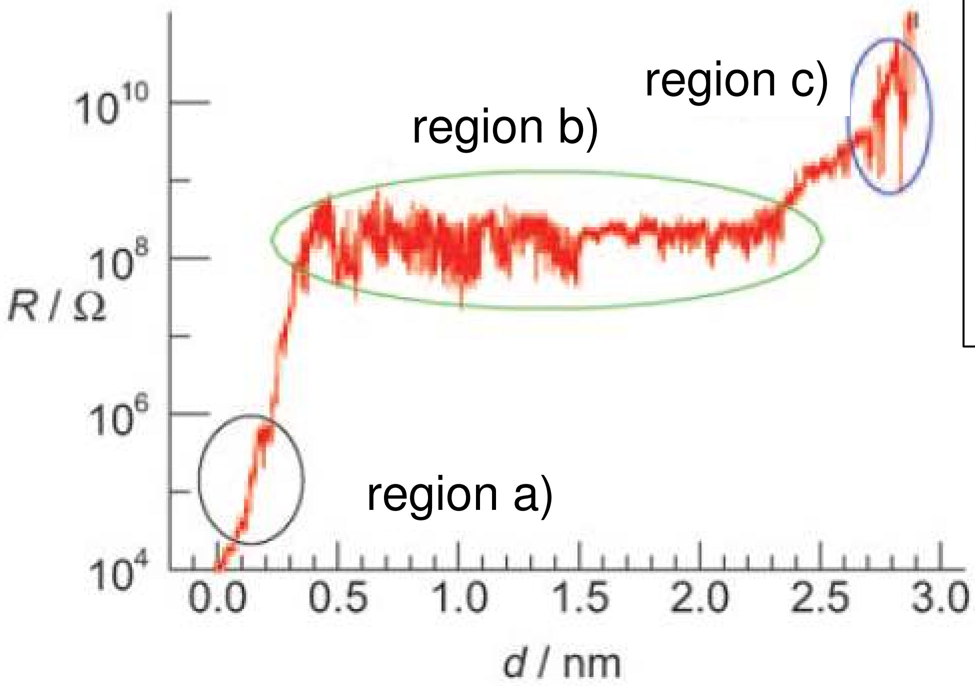


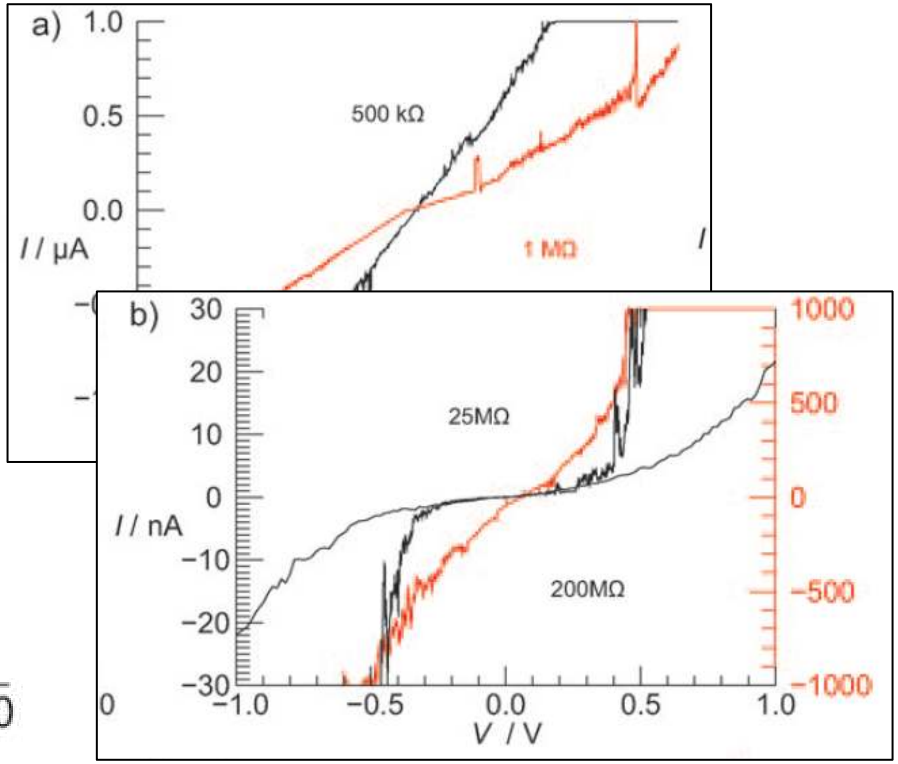


a) direct tunneling electrode-electrode

Transport through DNA quadruplexes

Resistance-distance dependence

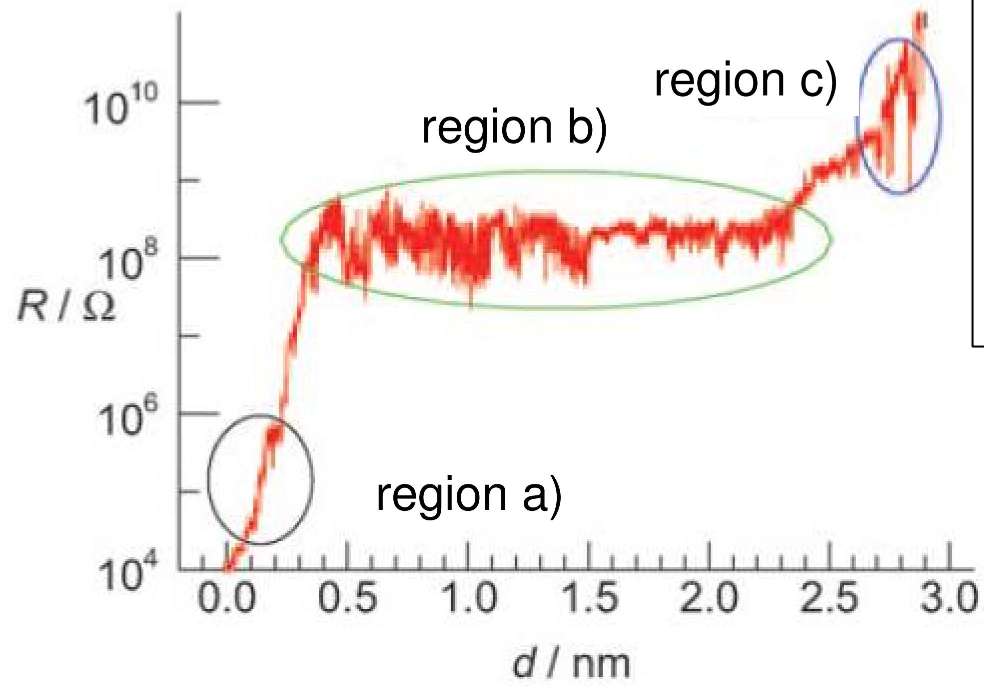


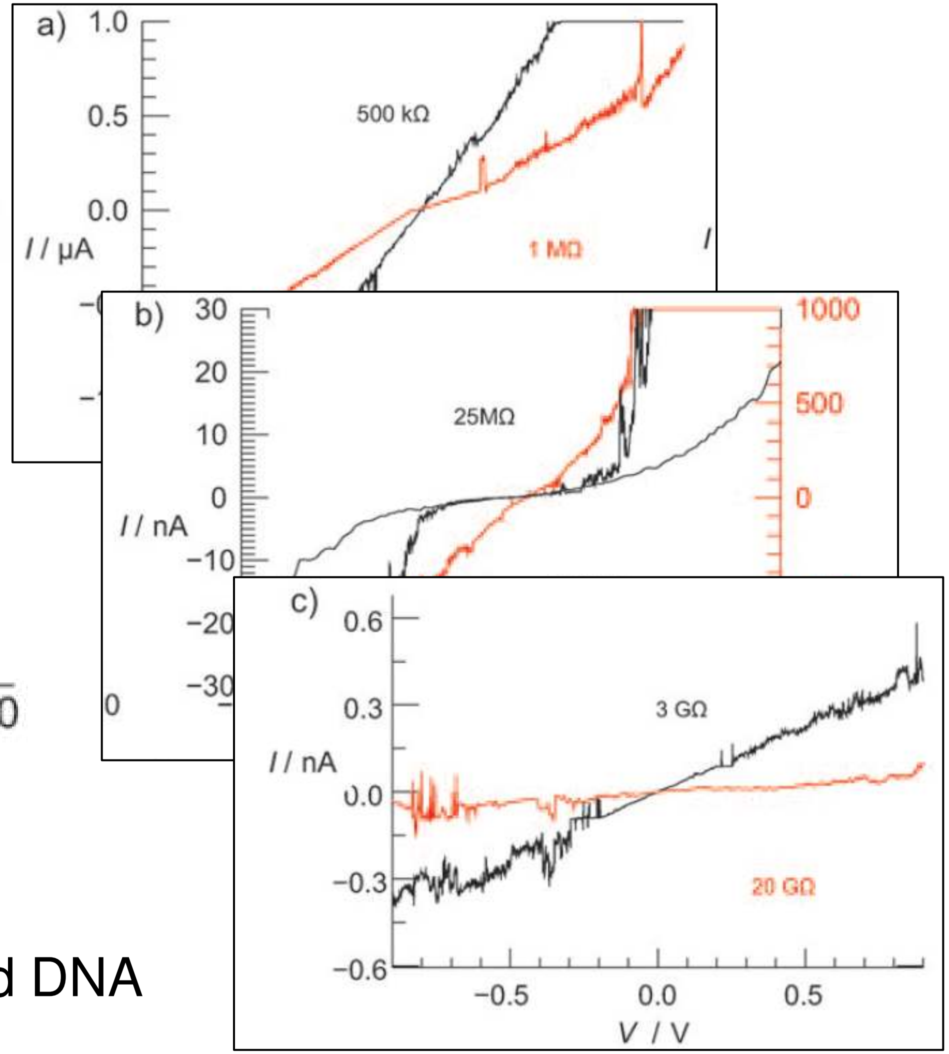


a) direct tunneling electrode-electrode
b) quadruplex unfolding

Transport through DNA quadruplexes

Resistance-distance dependence

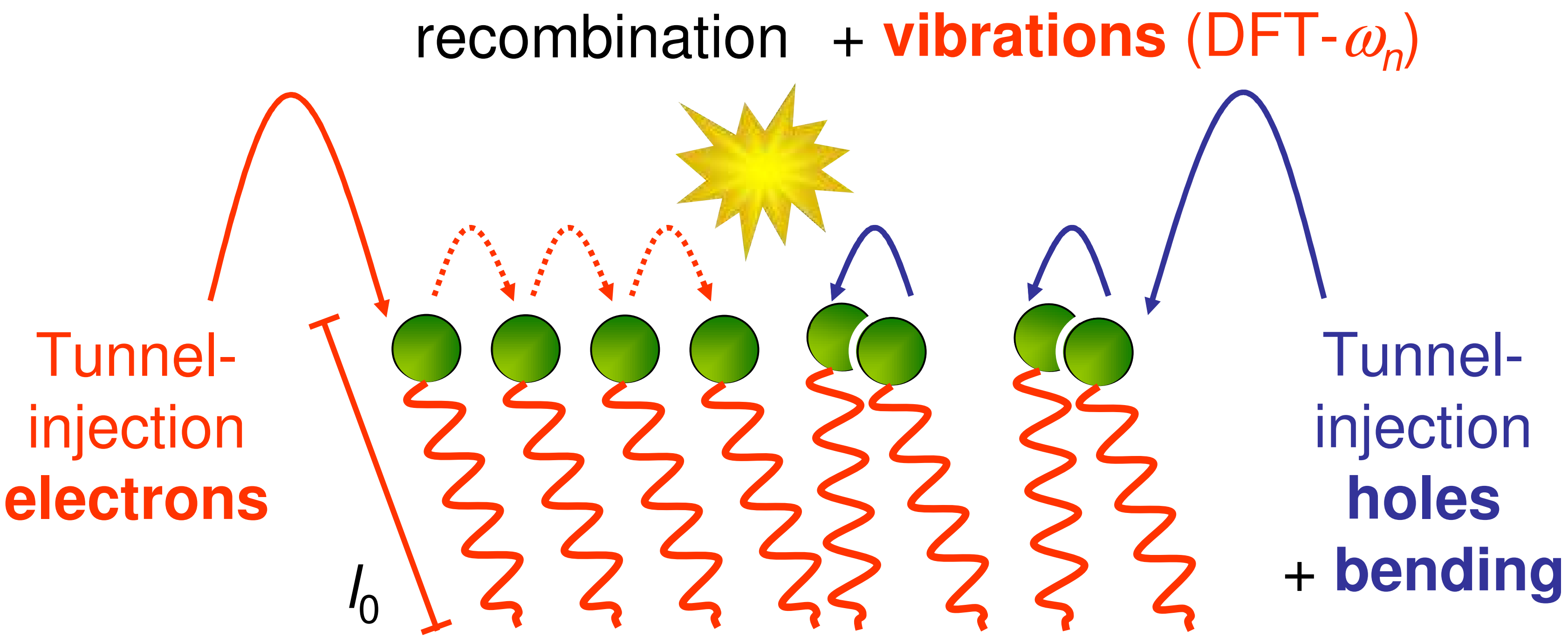




a) direct tunneling electrode-electrode
b) quadruplex unfolding
c) tunnel transport through single-strand DNA

Structure of Matter

Shuttling transport



continuum elasticity

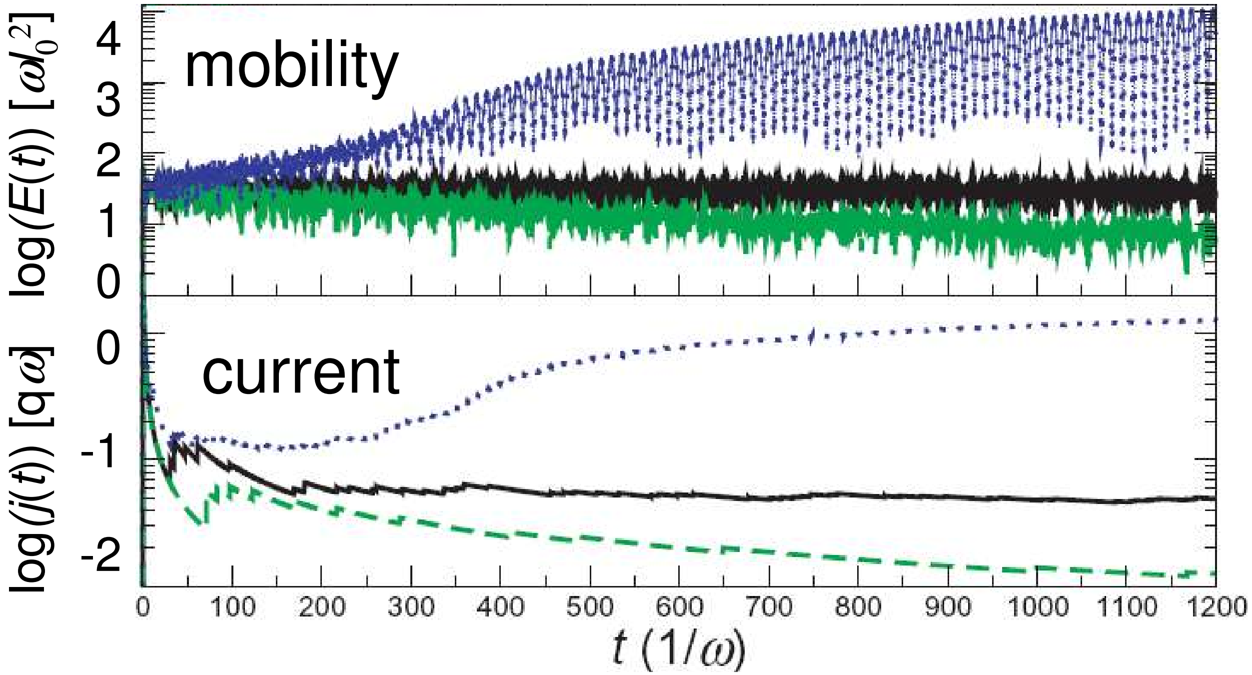
$$x_i(t) = \Sigma_n \phi_{ni} \left[(c_n \cos \omega_n t + d_n \sin \omega_n t) + \int_0^t dt' \left((\sin \omega_n (t-t')/\omega_n) \, \Sigma_m a_m(t') \phi_{nm} \right) \right]$$

transport equation

$$q_{i,\mathrm{nee}} = q_{i,\mathrm{old}} + \Delta q_{i,\mathrm{trans}} + \Delta q_{i,\mathrm{tunn}} - \Delta q_{i,\mathrm{rec}}$$

(normal basis: ϕ_{ni})

Shuttling transport – diode effect



bias voltage

-0.2 V = ↑↓ bending
no current

0.0 V = little current

0.2 V = ↑↑ bending
high current

New Journal of Physics
The open-access journal for physics

Current without external bias and diode effect in shuttling transport of nanoshafts

K Morawetz[1,2,3], S Gemming[1], R Luschtinetz[4], L M Eng[5], G Seifert[4] and A Kenfack[2]

current without bias

diode effect

dissipative effects assist or counteract

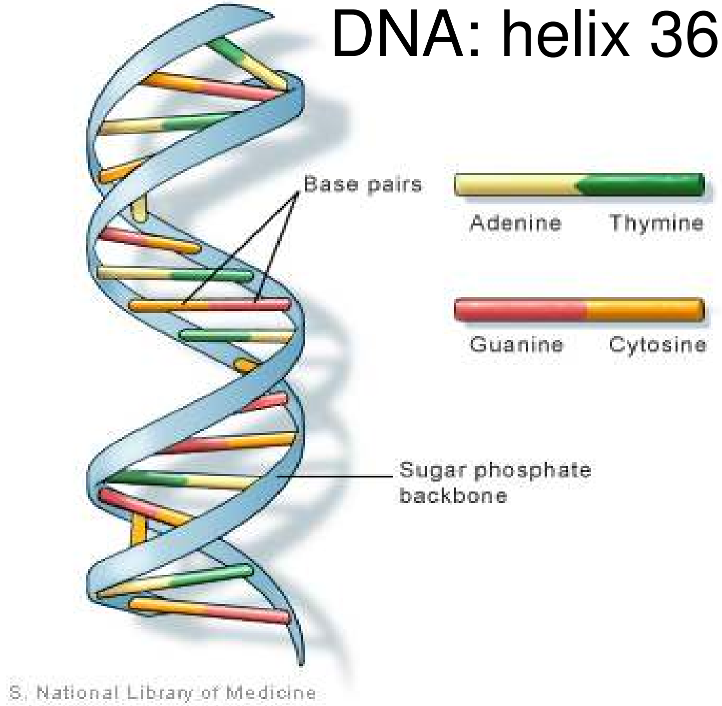
Continuous wire/tube gate

CNT@DNA

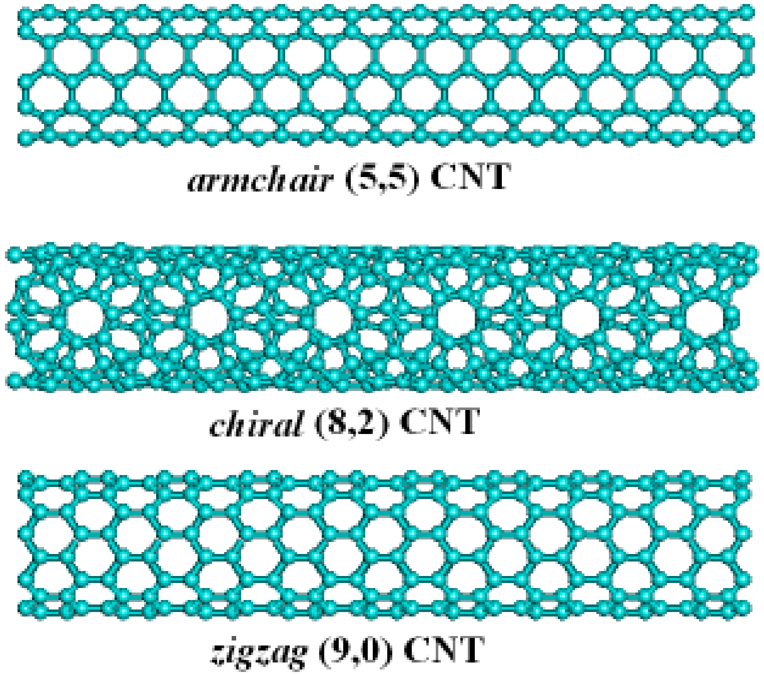
$(Mo_6S_6)_\infty$

CNT@DNA as Gate?

DNA: helix 36°



CNT – Winkel ~ Chiralität



IOP PUBLISHING NANOTECHNOLOGY

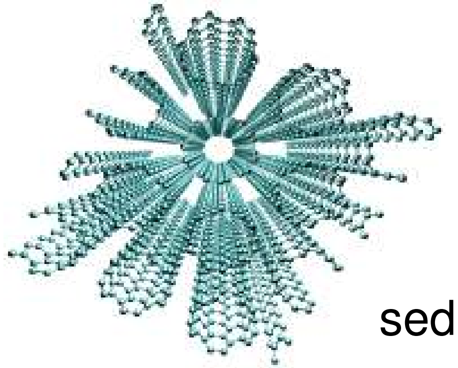
Nanotechnology **18** (2007) 245702 (10pp) doi:10.1088/0957-4484/18/24/245702

DNA-wrapped carbon nanotubes

A N Enyashin[1,2], S Gemming[3] and G Seifert[1]

Formation energy of CNT@DNA aggregates

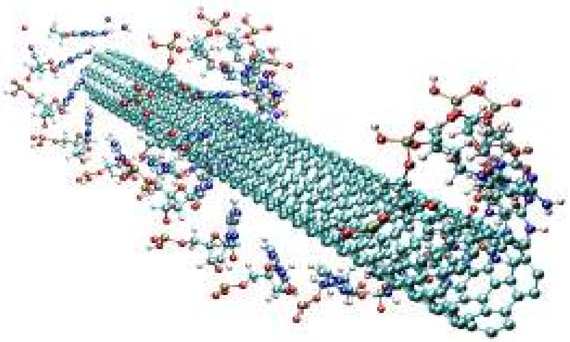
E_{coh} – cohesion of CNT bundles



CNT
sediment

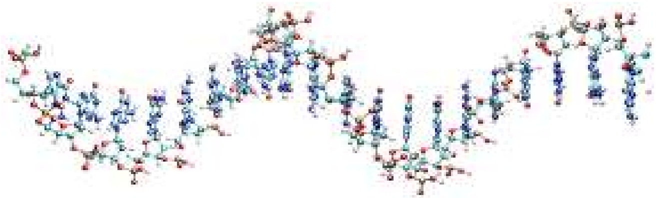
single CNT

E_{ads} – adsorption DNA – base on CNT

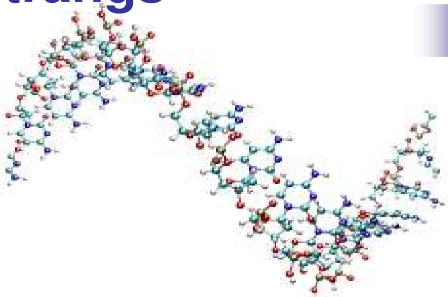


CNT@DNA complex

E_{def} – Deformation des DNA Strangs



ss-DNA molecule



distorted ss-DNA

ΔE_f – formation energy

Classical interaction model

first-principles
(DFT, HF-MP2)

E_{coh}, E_{def}, E_{int}

$$\Delta E_f = E_{coh} + NE_{def} + N_{base}E_{int}$$

analytic form

(N_{base}: number of bases)

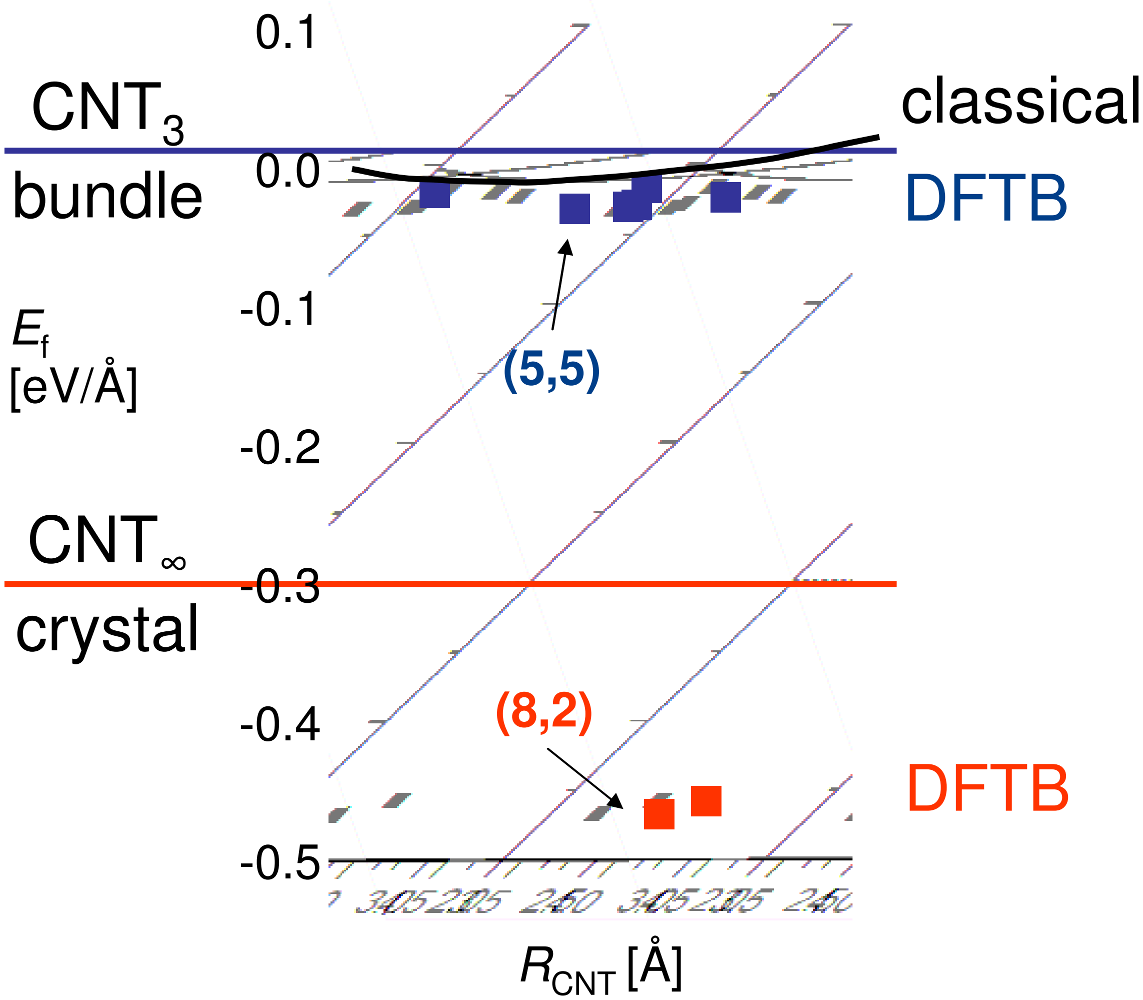
$$E_{coh} = a\sqrt{R_{CNT}}$$

$$E_{def} = a + b/(R_{DNA})^3 + cR_{DNA} + dR_{DNA}^2$$

$$R_{DNA} = R_{CNT} + l_{vdW} + l_{C\text{-}N}$$

(R: radius, N: number of DNA strands)

Validation vs. quantum mechanics: DFTB/disp

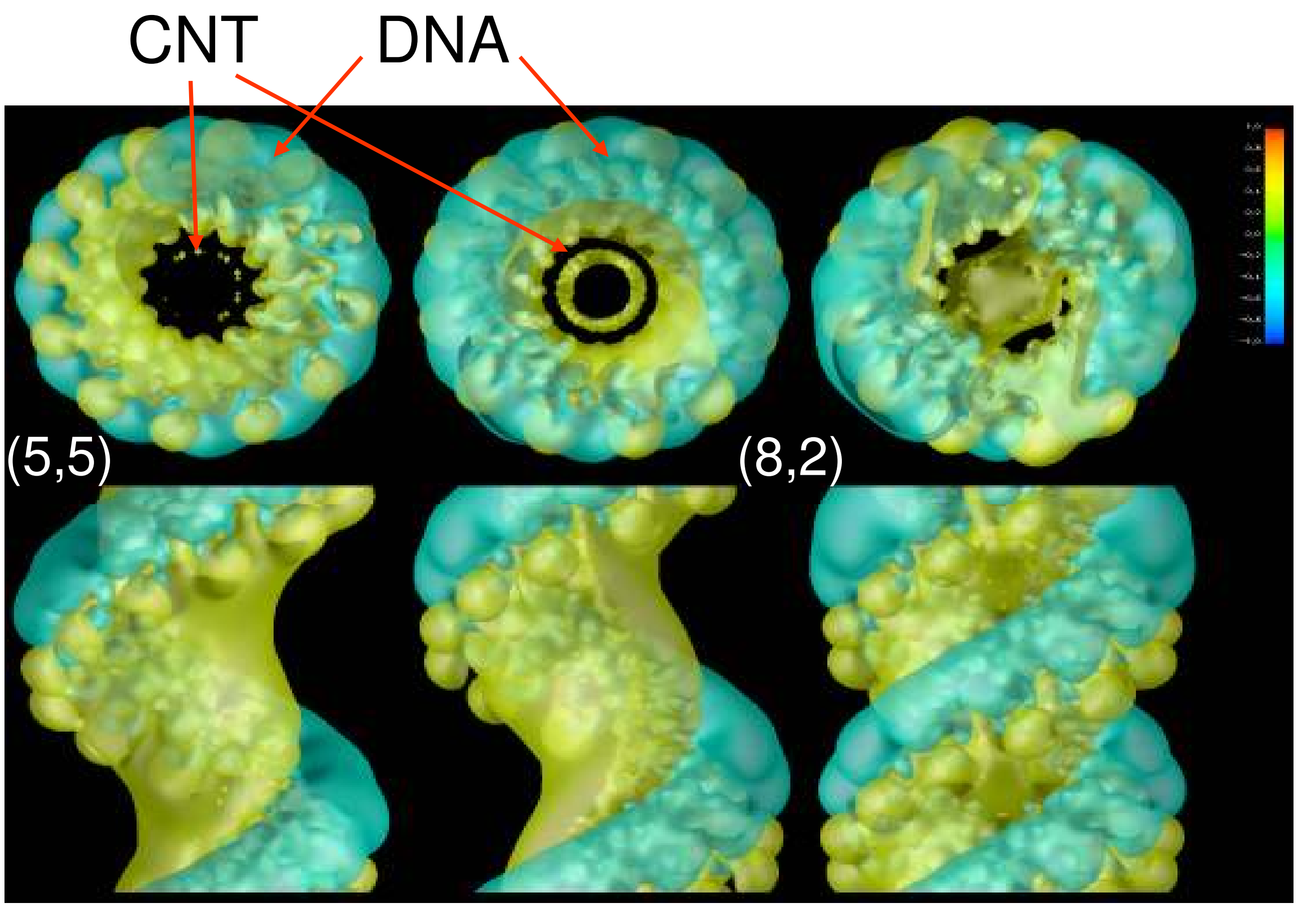


most cases
classical = QM

preferably
from CNT bundles
(sonicate!)

metallic & chiral CNT
stronger interaction

DF-TB – Charge transfer in CNT@DNA



electrostatic field: +0.4 e/Å (y) and -0.4 e/Å (b)

electron transfer

(5,5) @ poly-C: -0.005

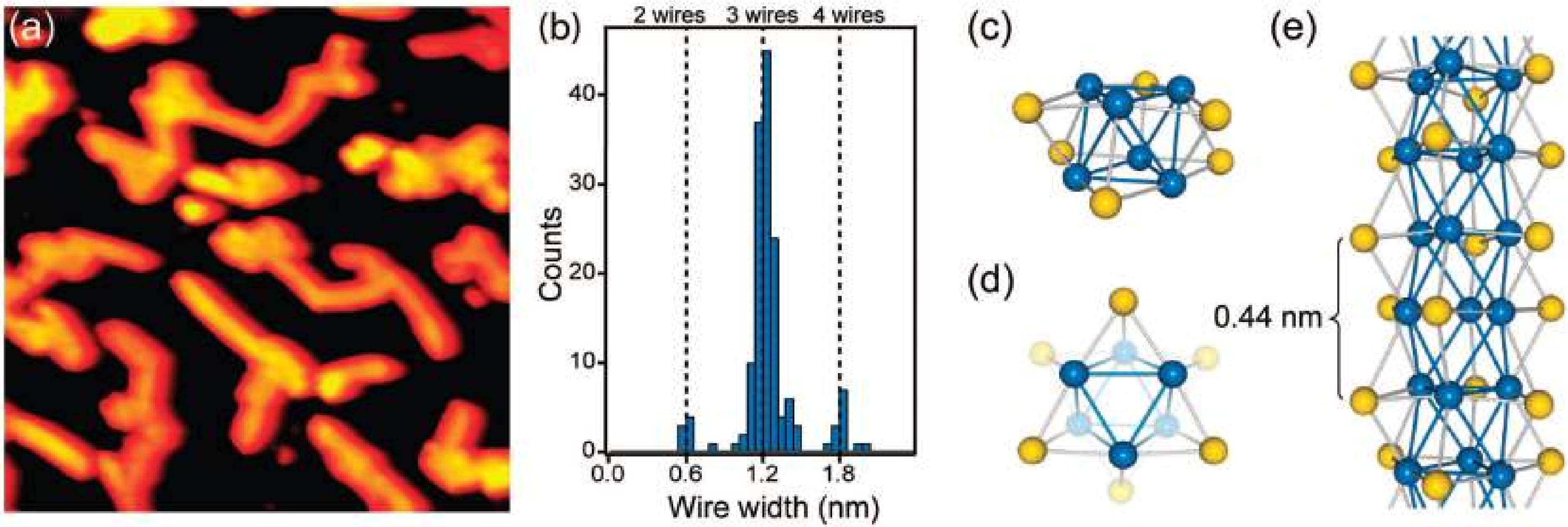
(8,2) @ poly-C: -0.374
2 poly-C: -0.825

(7,4) @ poly-C: -0.237

polar,
resonant transfer

ballistic transport

MoS_2 – based nanowires: S-deficient Mo_6S_6



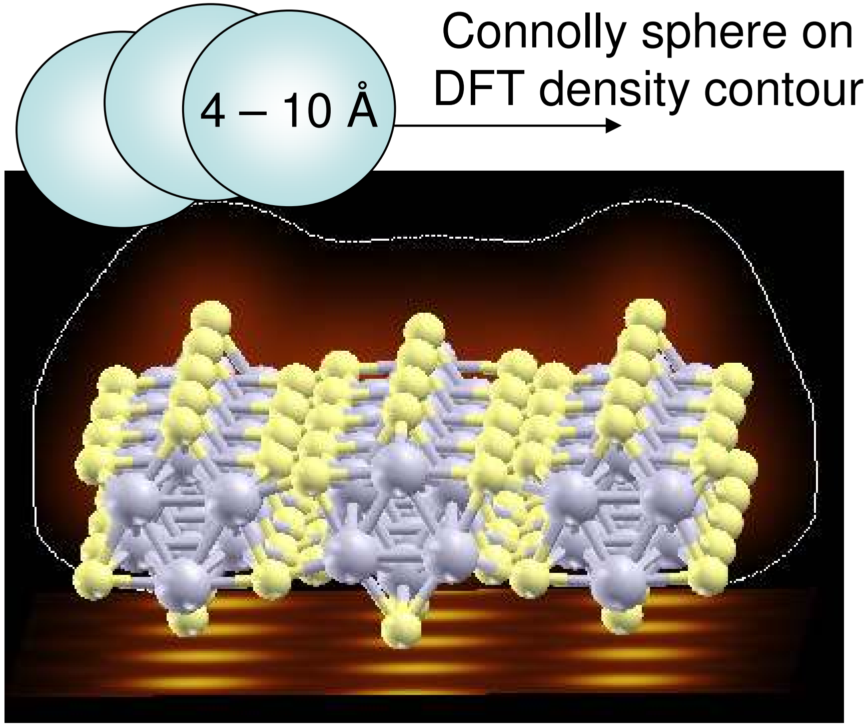
Atomic-Scale Structure of Mo_6S_6 Nanowires

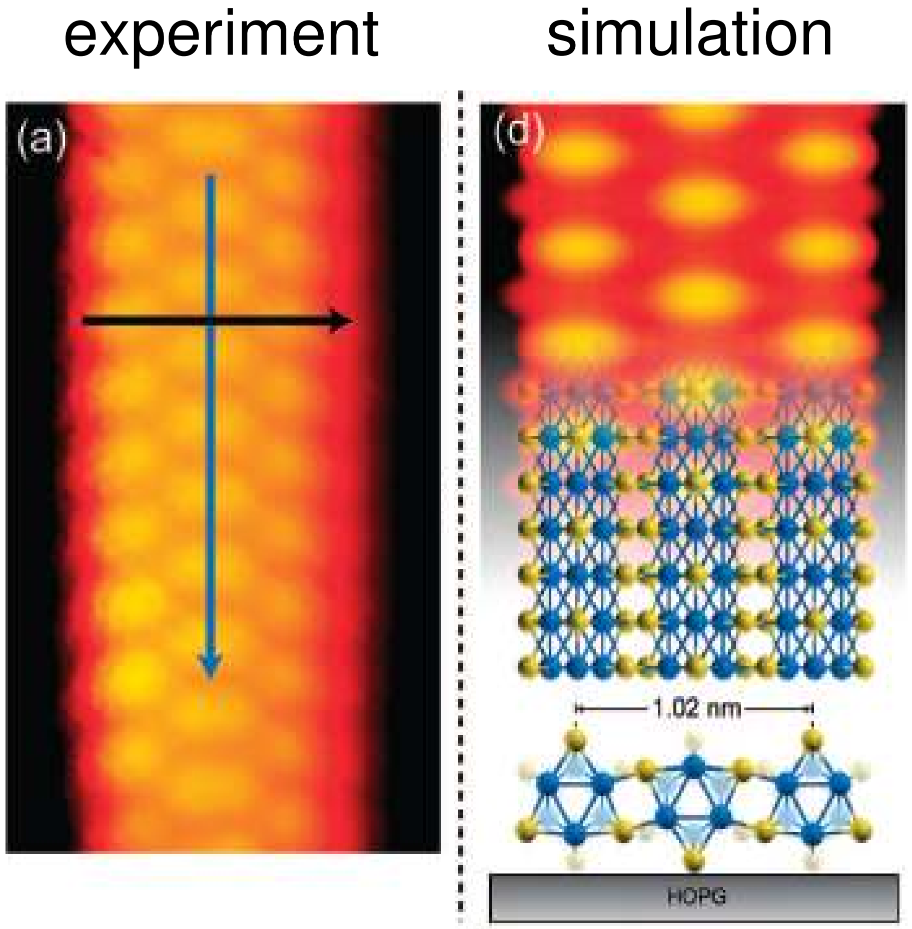
Jakob Kibsgaard,[†] Anders Tuxen,[†] Martin Levisen,[†] Erik Lægsgaard,[†] Sibylle Gemming,[‡] Gotthard Seifert,[§] Jeppe V. Lauritsen,[*,†] and Flemming Besenbacher[*,†]

NANO LETTERS

(*Nano Lett.* **8** (2008) 3928-3931)

Mo_6S_6 nanowires: STM - structure



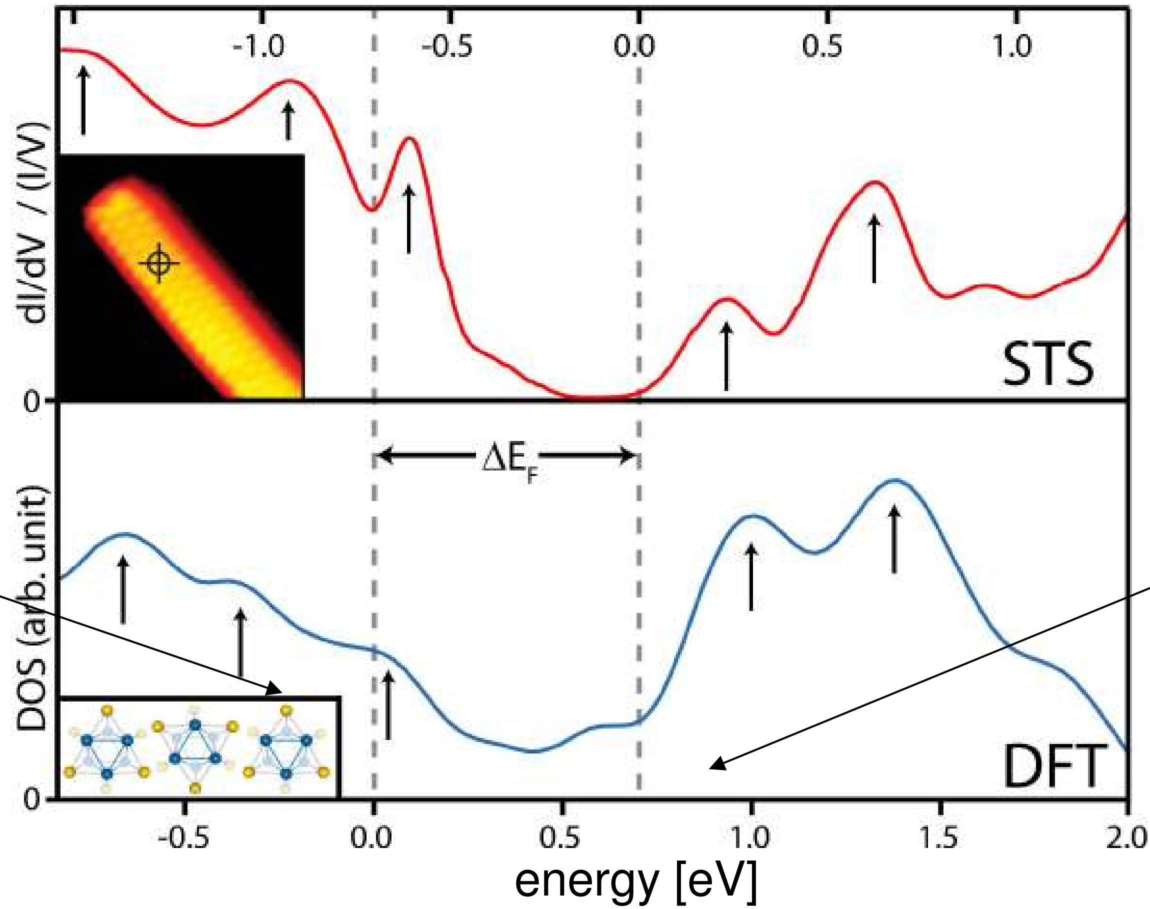


maxima at S
distances 4.4 Å, 10.2 Å
wire height 9.4(±0.1)Å

Structure of Matter

Mo_6S_6 nanowires: STS - conductivity

Mo *d*
+
S *p*
states

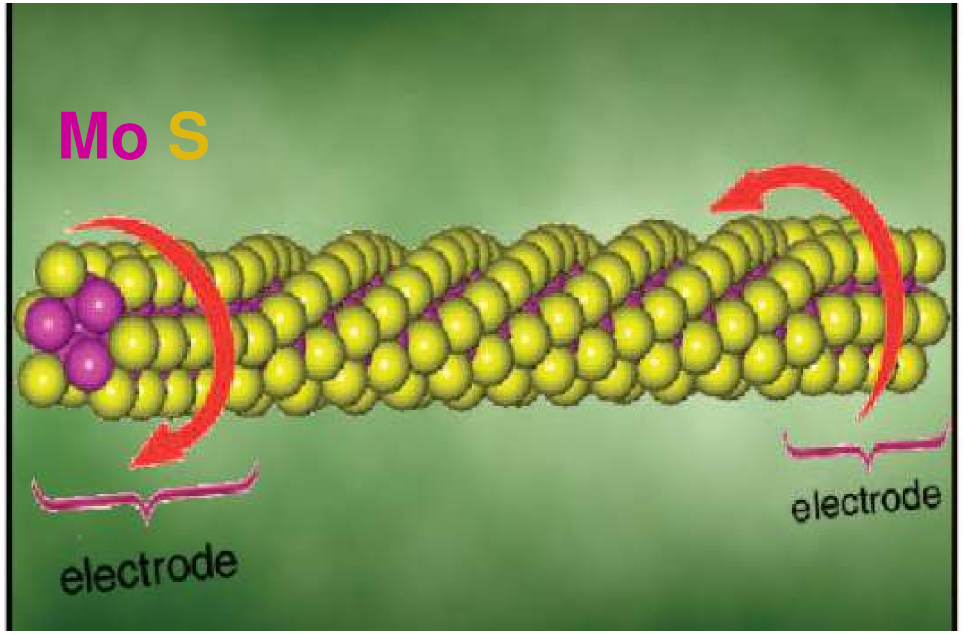


Mo *d*
states
=
conduction
band edge

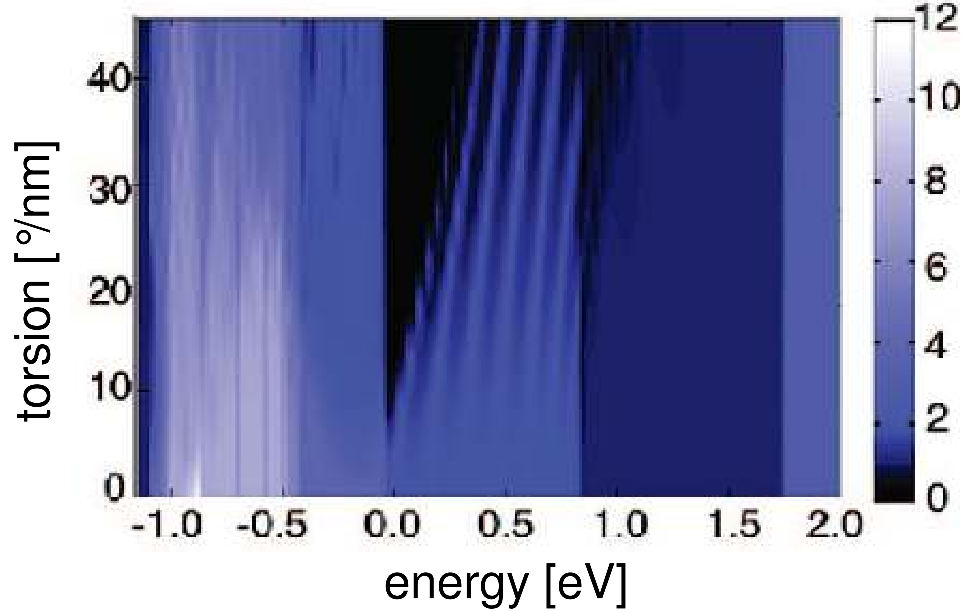
Besenbacher
(Aarhus)

metallic conductance through Mo part, S insulates

Mo_6S_6 : Electromechanic switch



DFPT: Transmission



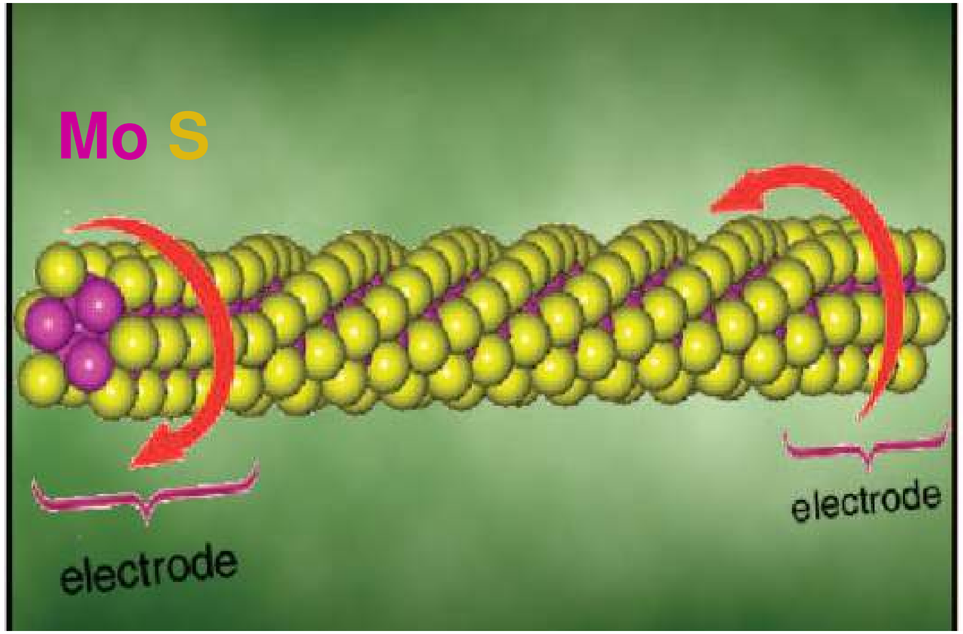
Electromechanical Switch Based on Mo_6S_6 Nanowires

Igor Popov,[*,†] Sibylle Gemming,[‡] Shinya Okano,[†] Nitesh Ranjan,[§] and Gotthard Seifert[†]

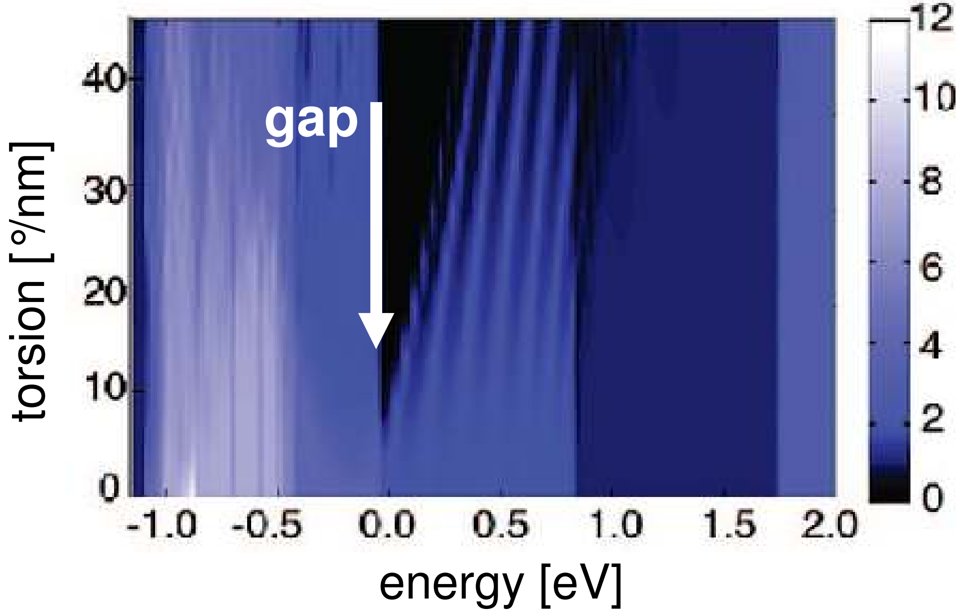
NANO LETTERS

(*Nano Lett.* **8** (2008) 4093-4097)

Mo_6S_6 : Electromechanic switch



DFPT: Transmission



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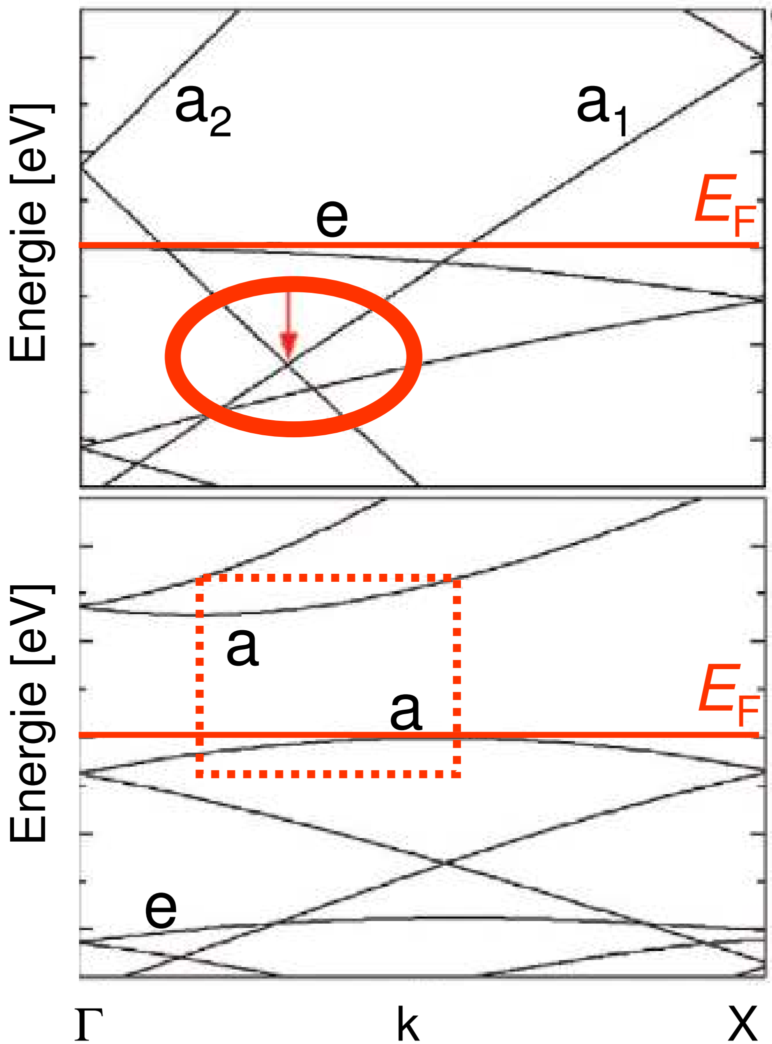
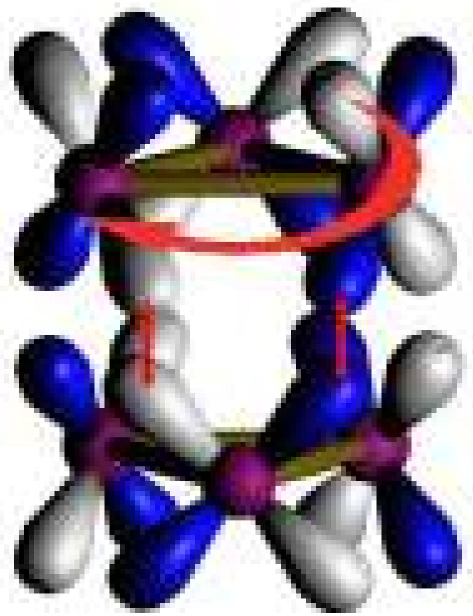
NANO LETTERS

(*Nano Lett.* **8** (2008) 4093-4097)

Mo_6S_6 : Structure-induced metal-insulator transition!





ideal: $\mathbf{C_{3v}}$

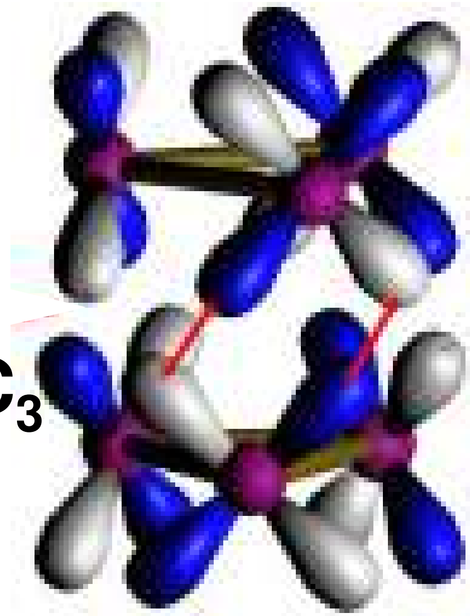
allowed

a_1-a_2-crossing

distorted: $\mathbf{C_3}$

forbidden

a-a-crossing



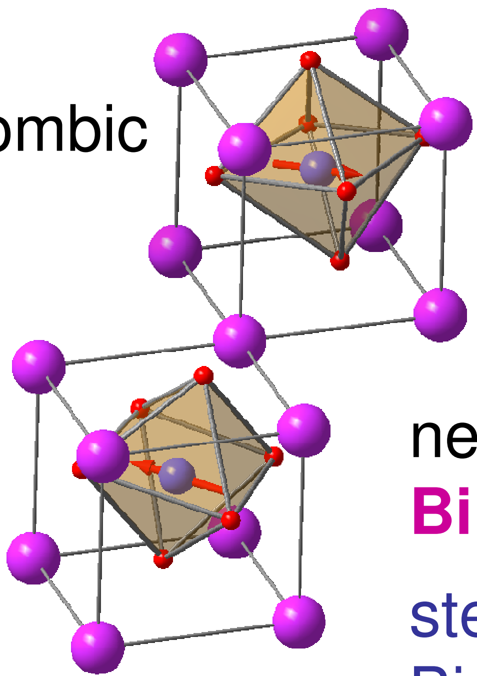
Switching – Electrostatic field on interfaces

Domain walls in $BiFeO_3$

Electrostatic field at domain boundaries

$BiFeO_3$

orthorhombic unit cell



tilted FeO_6 octahedra

near-cubic **Bi** arrangement

stereoactive Bi lone pair

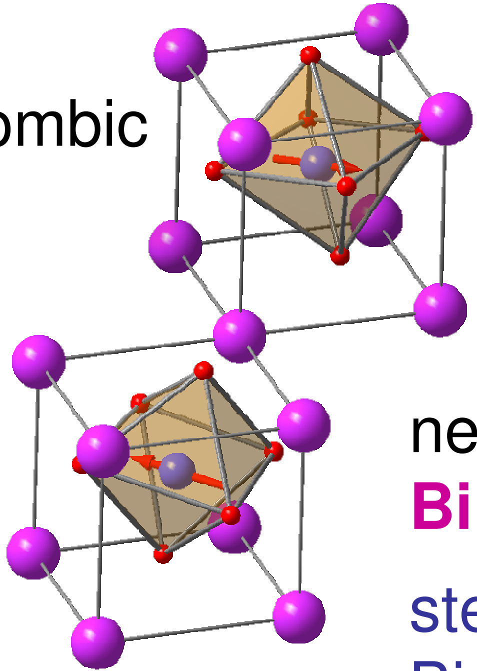
Conduction at domain walls in oxide multiferroics

J. Seidel[1,2*†], L. W. Martin[2,3*], Q. He[1], Q. Zhan[2], Y.-H. Chu[2,3,4], A. Rother[5], M. E. Hawkridge[2], P. Maksymovych[6], P. Yu[1], M. Gajek[1], N. Balke[1], S. V. Kalinin[6], S. Gemming[7], F. Wang[1], G. Catalan[8], J. F. Scott[8], N. A. Spaldin[9], J. Orenstein[1,2] and R. Ramesh[1,2,3]

Electrostatic field at domain boundaries

$BiFeO_3$

orthorhombic
unit cell



tilted
FeO_6
octahedra

near-cubic
Bi arrangement

stereoactive
Bi lone pair

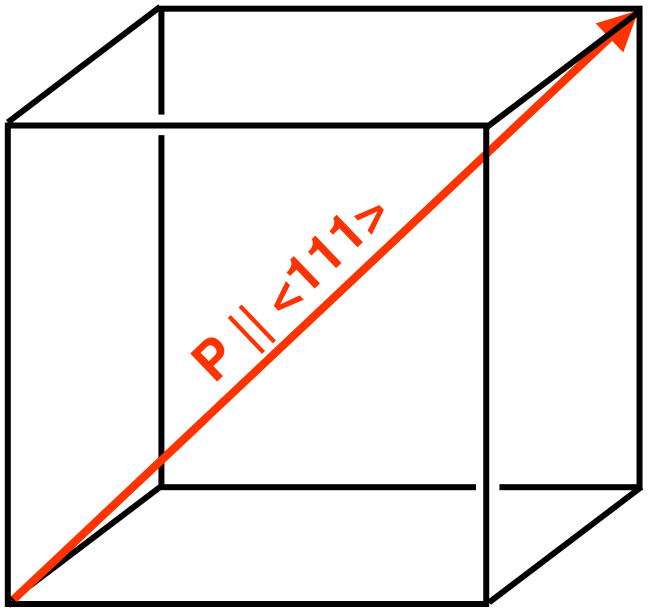
- antiferromagnet
  T_N ~ 650 K
- rhombohedral ferroelectric
  T_C ~ 1103 K
- spontaneous polarization
  P ~ 90 C cm^{-2}
  along pseudocubic <111>

nature materials

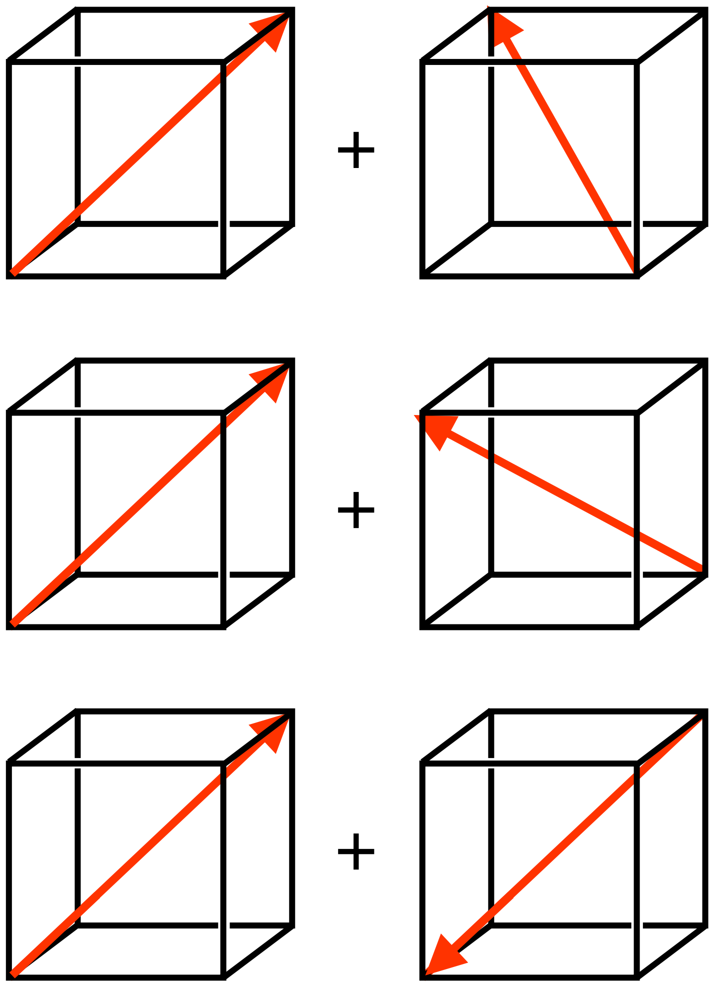
Conduction at domain walls in oxide multiferroics

J. Seidel[1,2*†], L. W. Martin[2,3*], Q. He[1], Q. Zhan[2], Y.-H. Chu[2,3,4], A. Rother[5], M. E. Hawkridge[2], P. Maksymovych[6], P. Yu[1], M. Gajek[1], N. Balke[1], S. V. Kalinin[6], S. Gemming[7], F. Wang[1], G. Catalan[8], J. F. Scott[8], N. A. Spaldin[9], J. Orenstein[1,2] and R. Ramesh[1,2,3]

Relative domain orientations



ferroelectric
polarization
P || <111>

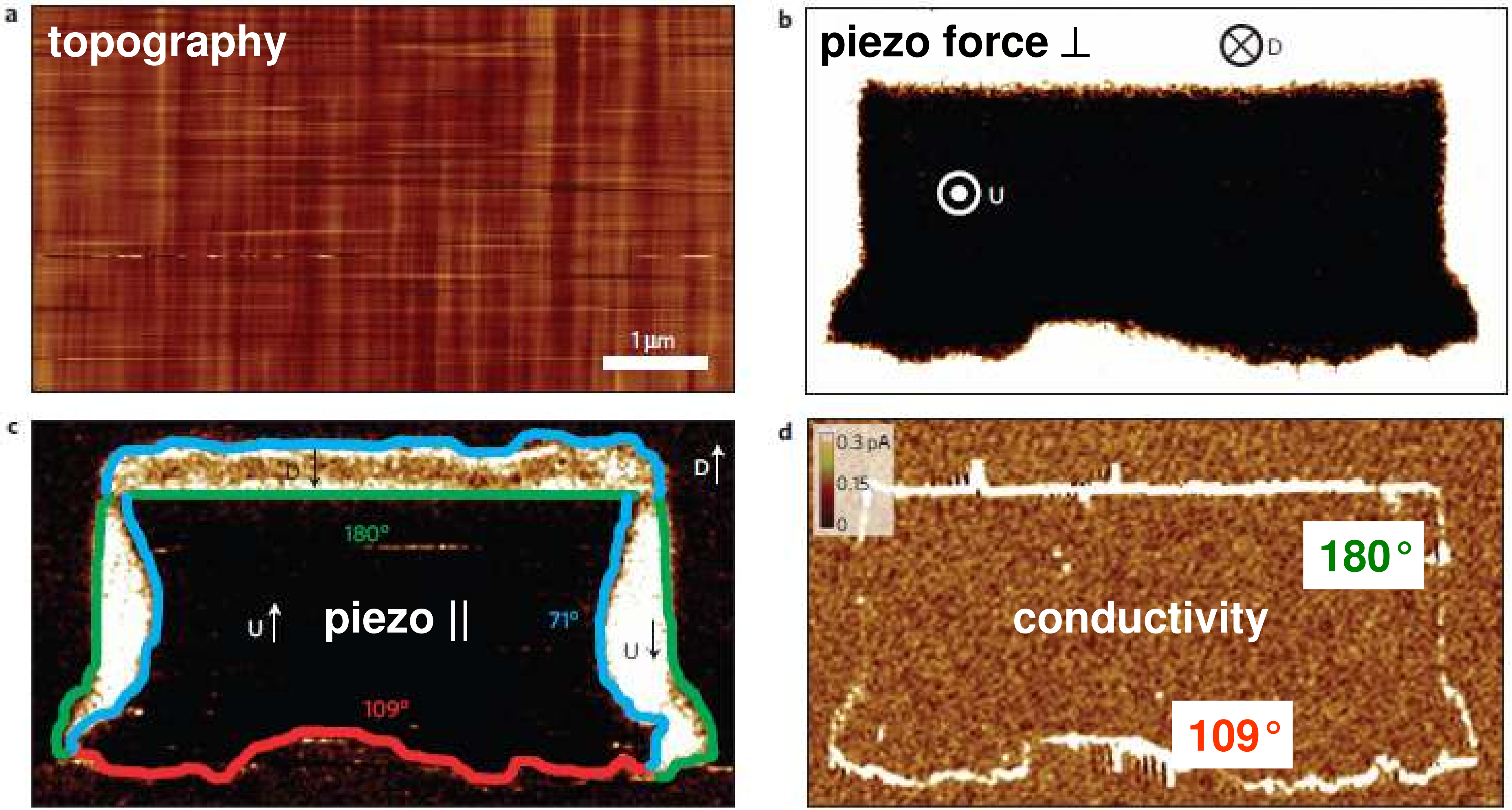


71° wall

109° wall

180° wall

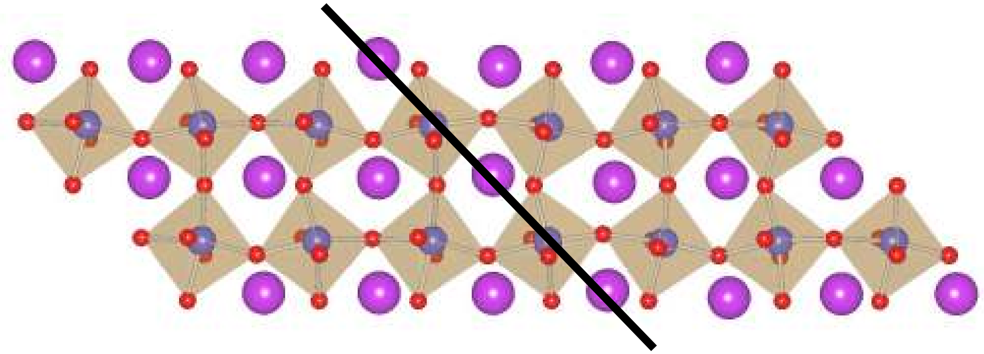
Observed domain walls



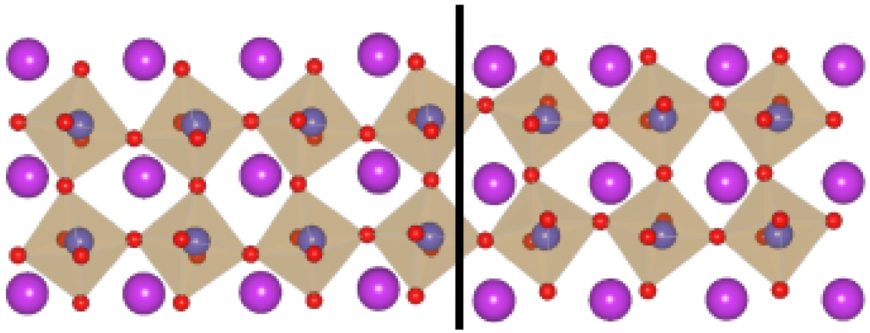
71 ° 109 ° 180 °

Domain wall structures

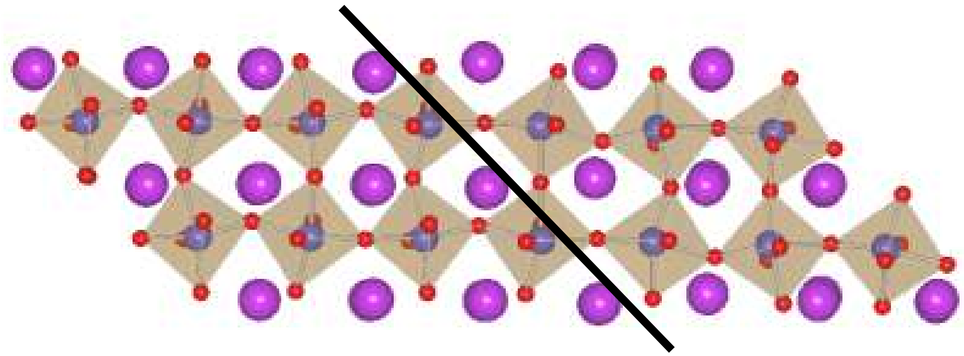
71° wall



109° wall

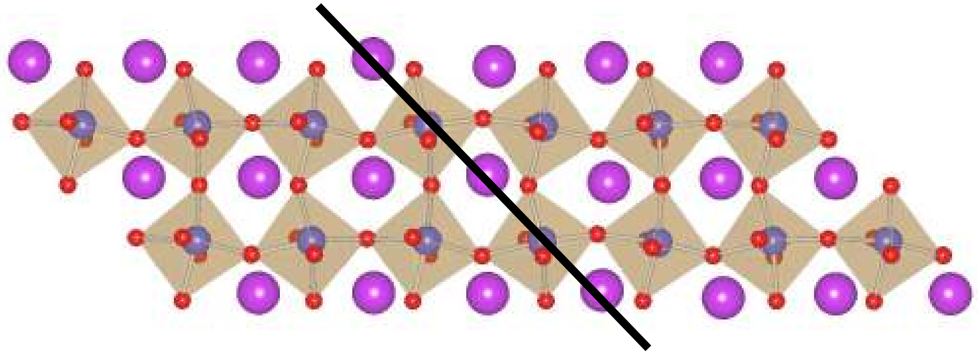


180° wall



Domain wall structures – electronic structure

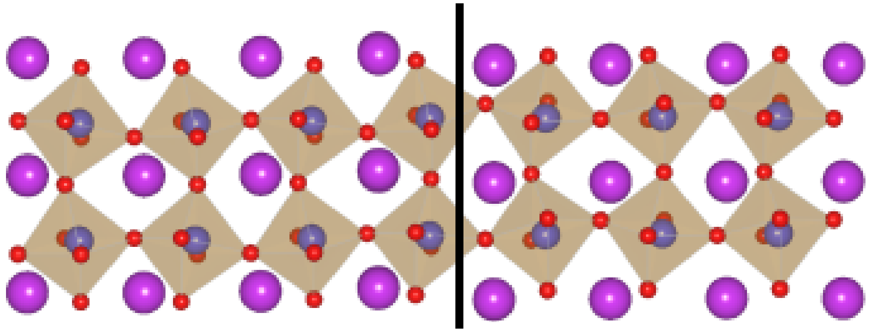
71 ° wall



E_D = 0.36 J/m²
ΔV = 0.02 eV
ΔE_g = -0.05 eV

109 ° wall

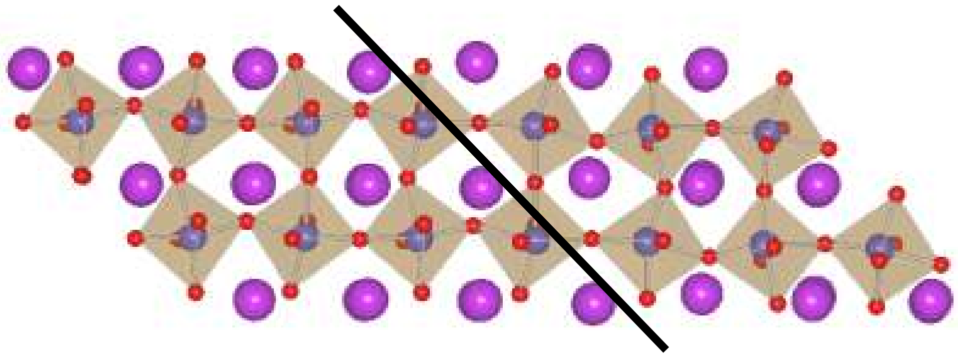
very stable
conducting!



E_D = 0.21 J/m²
ΔV = 0.18 eV
ΔE_g = -0.20 eV

180 ° wall

conducting!



E_D = 1.81 J/m²
ΔV = 0.15 eV
ΔE_g = -0.10 eV

Conclusions

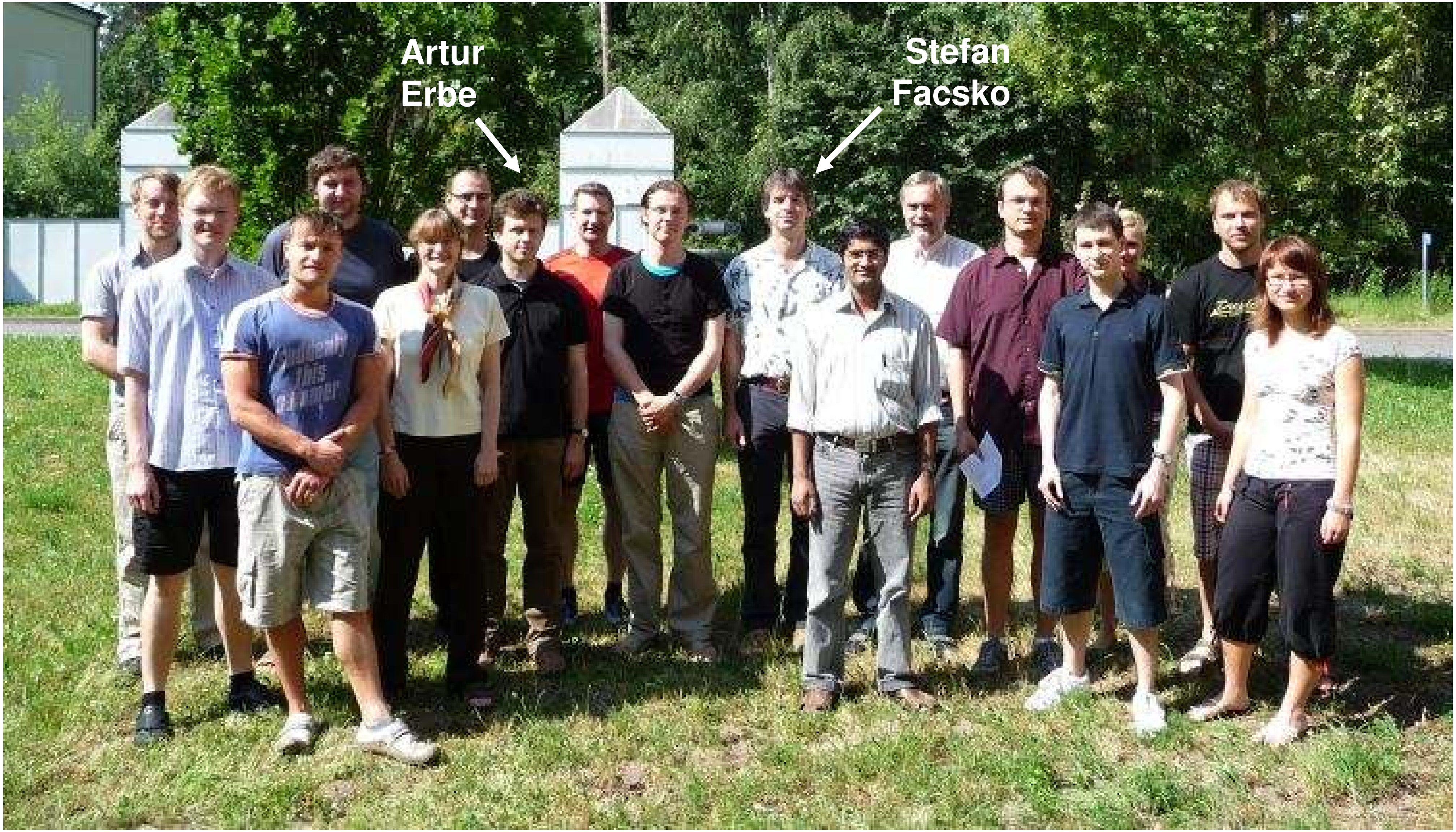
- Hopping transport
  - Parameter transfer first-principle to classical transport
  - Transport without bias by shuttling
- Ballistic transport
  - Model derivation from first-principles data
  - Elastomechanic metal-insulator transition
- Transport at defects in the bulk
  - Existence of strong surface/interface polarizations
  - Origin of conductivity at domain walls

Thanks

Structure of Matter

Thanks

Structure of Matter



Thanks

Structure of Matter

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N. Spaldin (Santa Barbara)

§ Euros

DFG, BMBF, DAAD, GIF

Thank you!

Forschungszentrum
Dresden Rossendorf

Transition metal - chalcohalide MX_2

DFG, SP … Konstanz;

Titanate-defect phases

DFG, 11/07-04/09, 0.5
D. Meyer, TUD,
T. Gemming, IFW

Manganates ($RMnO_3$, R_2MnO_5)

Pakt, 01/06-12/08, 1.0,
Novak, Prag

+ MC

Transport

Electronics

Nanomagnets, DMS (V:Si, Co:TiO_2)

FZD, J. Wosnitza

+ moled

Density-Functional-Theory

Ferroic organic field effect transistor

SPP 11…
G. Seit…

Elastomagnetics (Co,Pd)|piezo

FOR 520, 07/06-06/09, 0.75;
Sächs. Exzellenz., 01/09-12/12, 1.5

Structure - Dimension

+ phase field

Scale-bridging modeling of bio-nano-boundaries

SPP 1155, 10/05-12/09, 0.5; DFG/BMBF 10/08-12/11, 0.75, RWTH Aachen