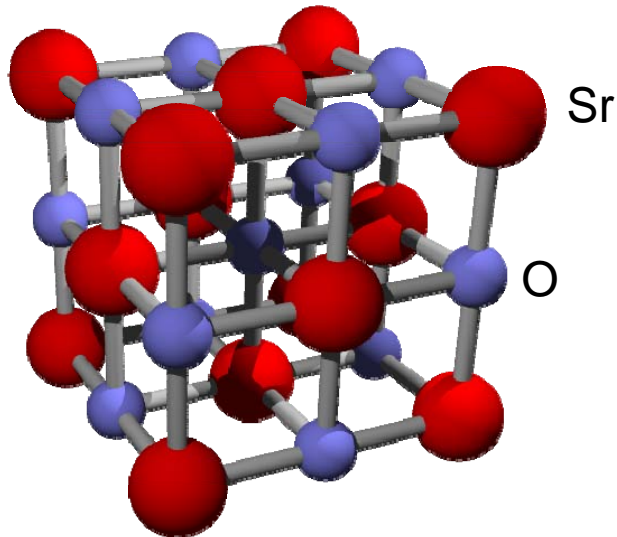


# Arbeitsgebiete AG Pfnür

1. Epitaktische Isolatorschichten
2. Neuartige  
Strukturierungsverfahren
3. Metallische Nanodrähte
4. Molekulare Elektronik

# Ultradünne, kristalline dielektrische Schichten: die Suche nach neuen Gate-Dielektrika

SrO



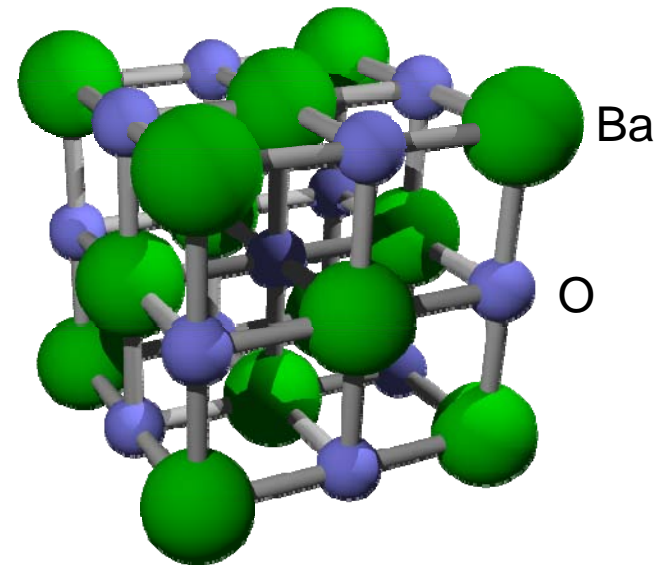
$$a_0 = 5.16 \text{ \AA}$$

$$\epsilon_r = 13.3$$

$$E_G = 6.4 \text{ eV}$$

NaCl-lattice

BaO



$$a_0 = 5.54 \text{ \AA}$$

$$\epsilon_r = 34$$

$$E_G = 4.4 \text{ eV}$$

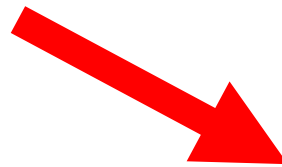
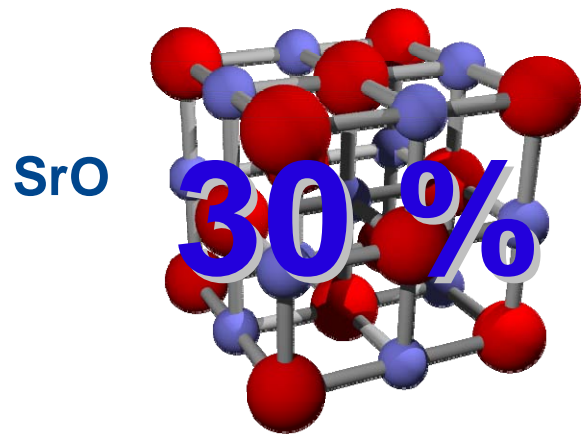
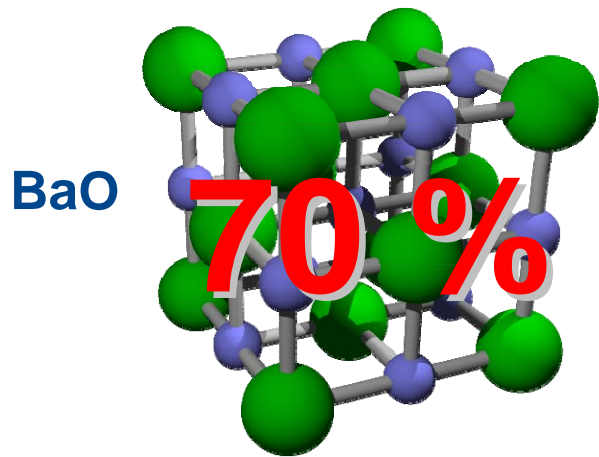
NaCl-lattice

$$a_0 (\text{Si}) = 5.43 \text{ \AA}$$

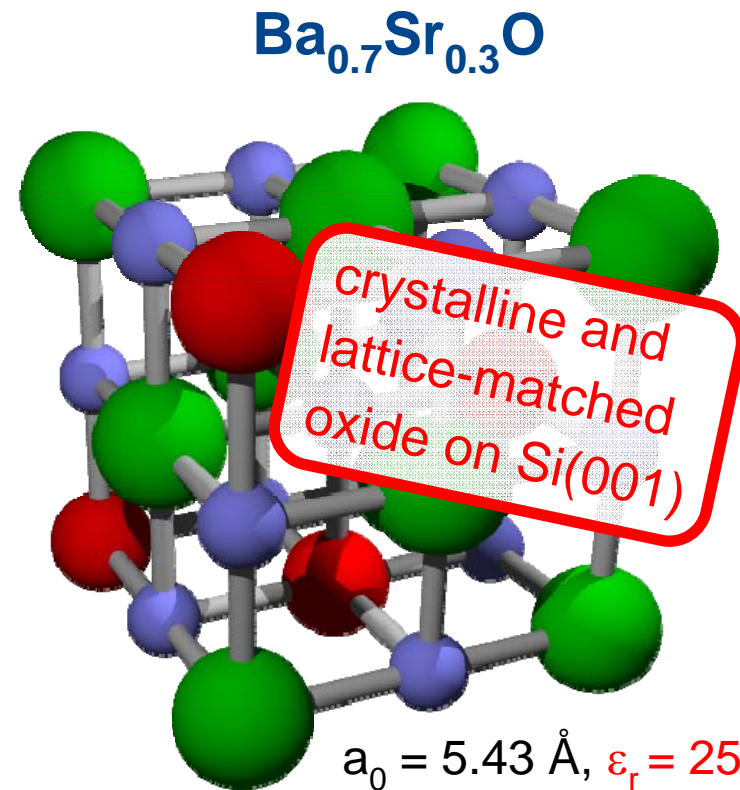
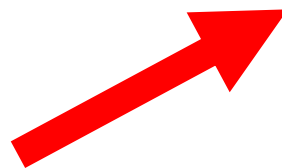
$$\epsilon_r (\text{SiO}_2) = 3.9$$

$$E_G (\text{SiO}_2) = 8.9 \text{ eV}$$

amorphous (SiO<sub>2</sub>)



mixing

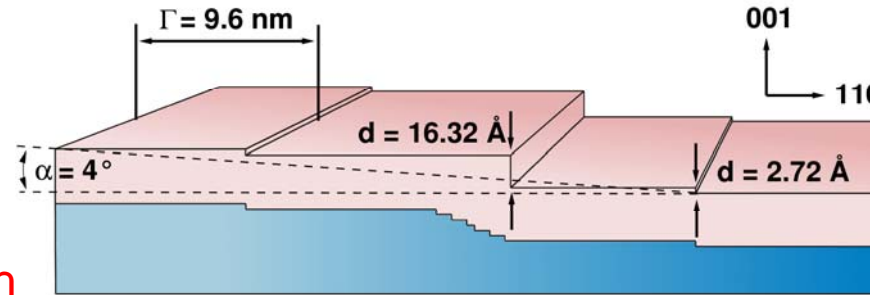


$a_0 = 5.43 \text{ \AA}$ ,  $\epsilon_r = 25-30$ ,  
 $E_G = 4.3 \text{ eV}$ , NaCl lattice

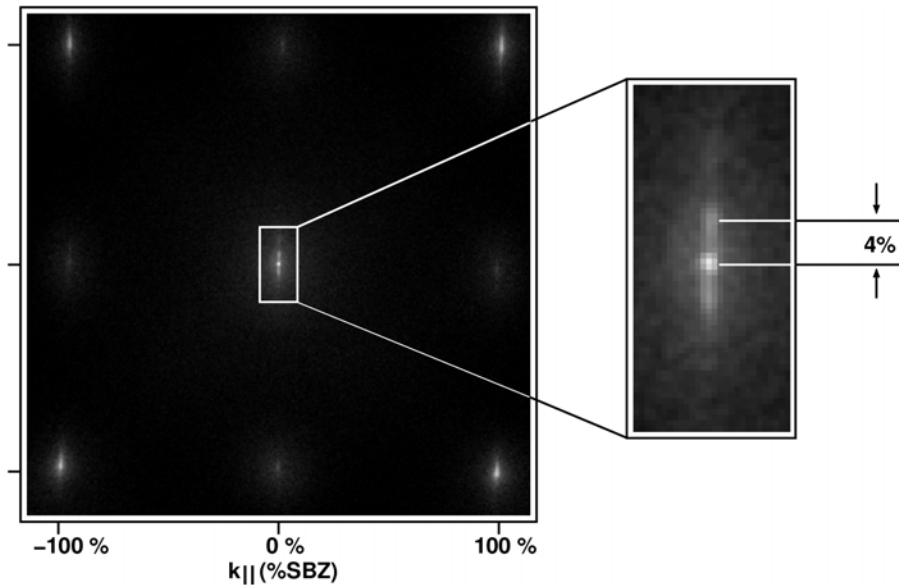
# Growth of vicinal BaO/SrO layers

10ML Ba<sub>0.7</sub>Sr<sub>0.3</sub>O

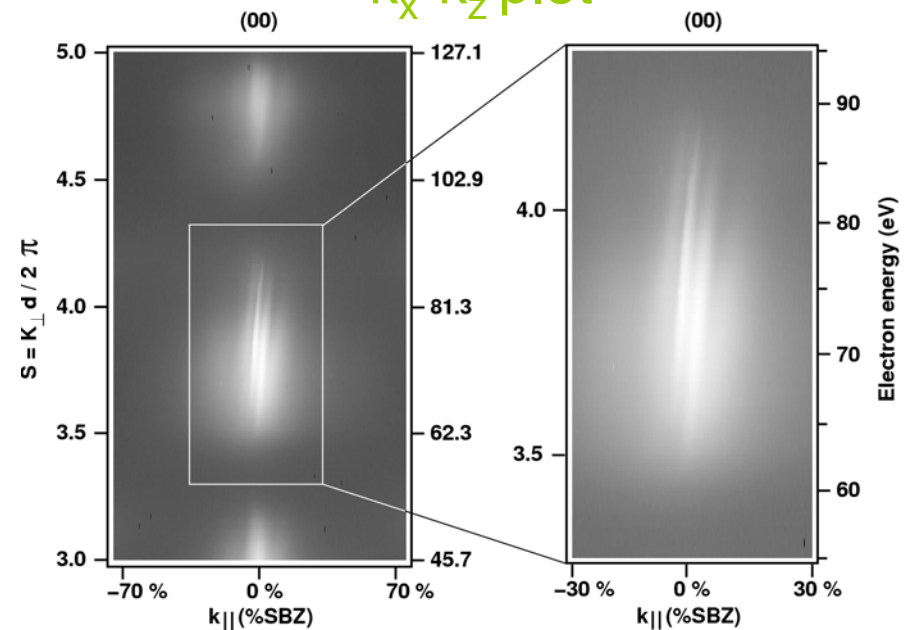
- (nominally) polar step formation
- critical step density for overgrowth of steps



$k_x$ - $k_y$  plot



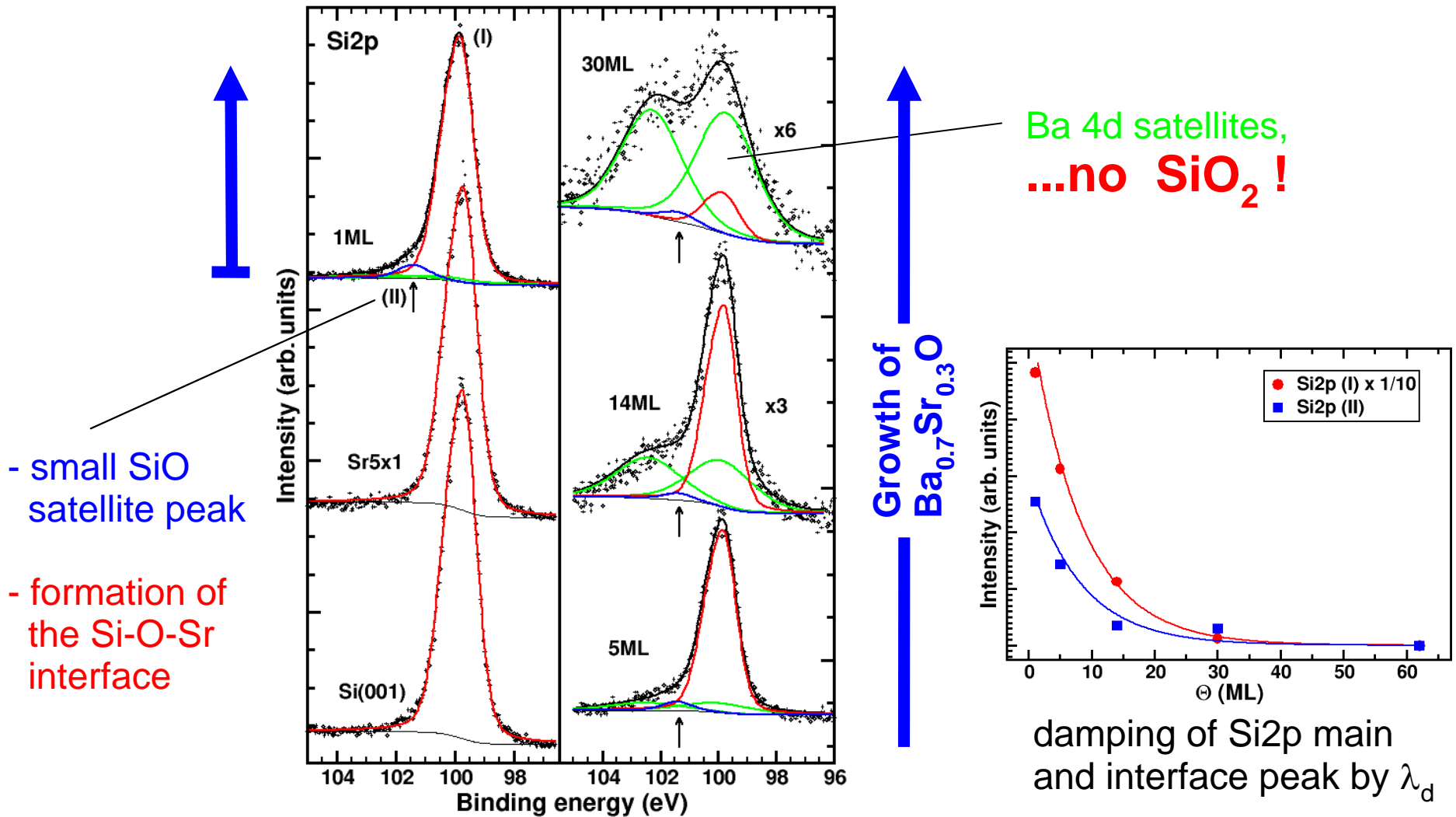
$k_x$ - $k_z$  plot



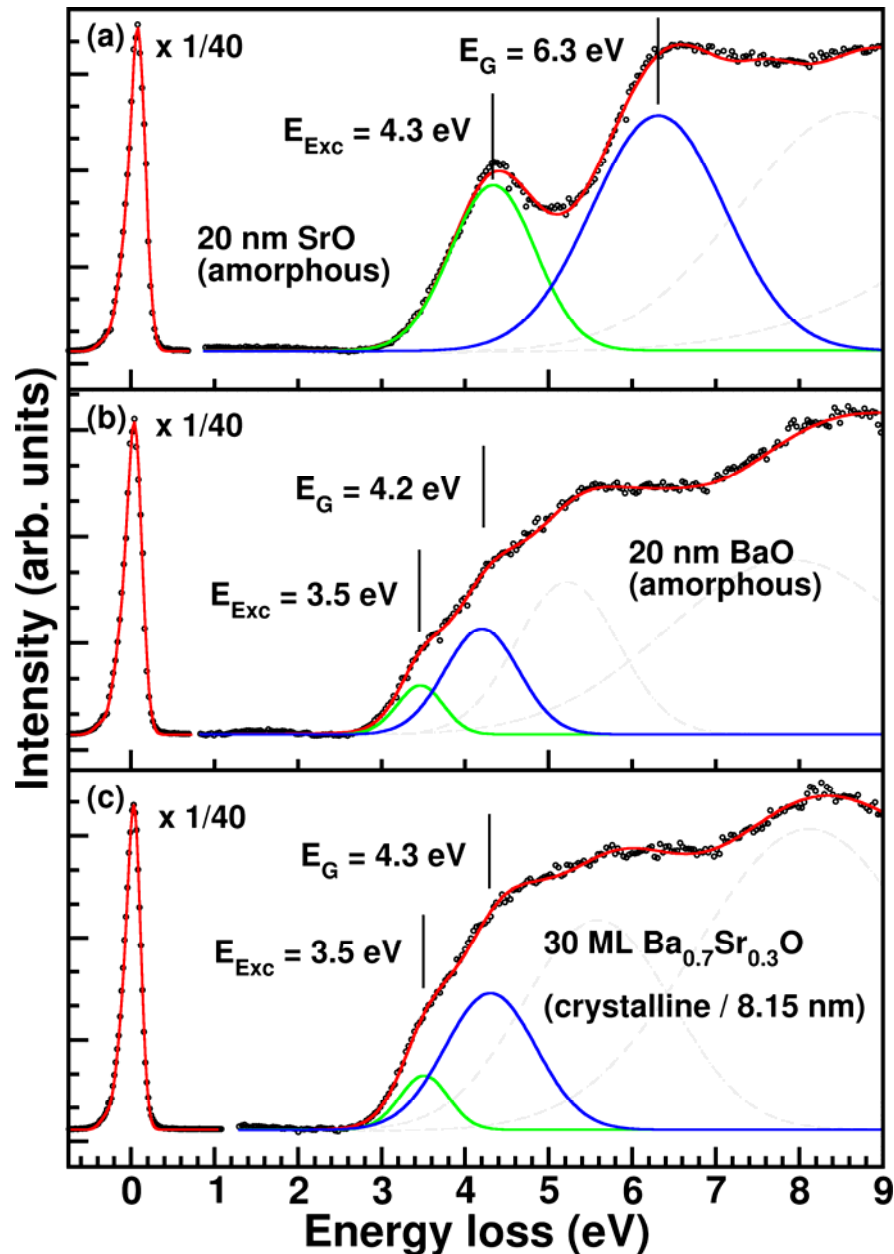
J. Zachariae and H. Pfnür, Surf. Sci. 600 (2006) 2785

# Chemical analysis of the interface

## XPS-measurement of the Si2p-spectra

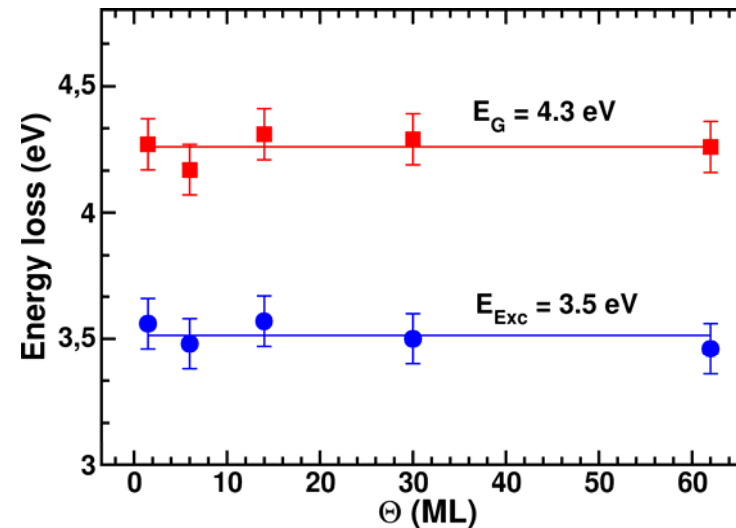


# Electronic structure: Band gap and excitonic



EELS-spectra of band gap and excitonic structure

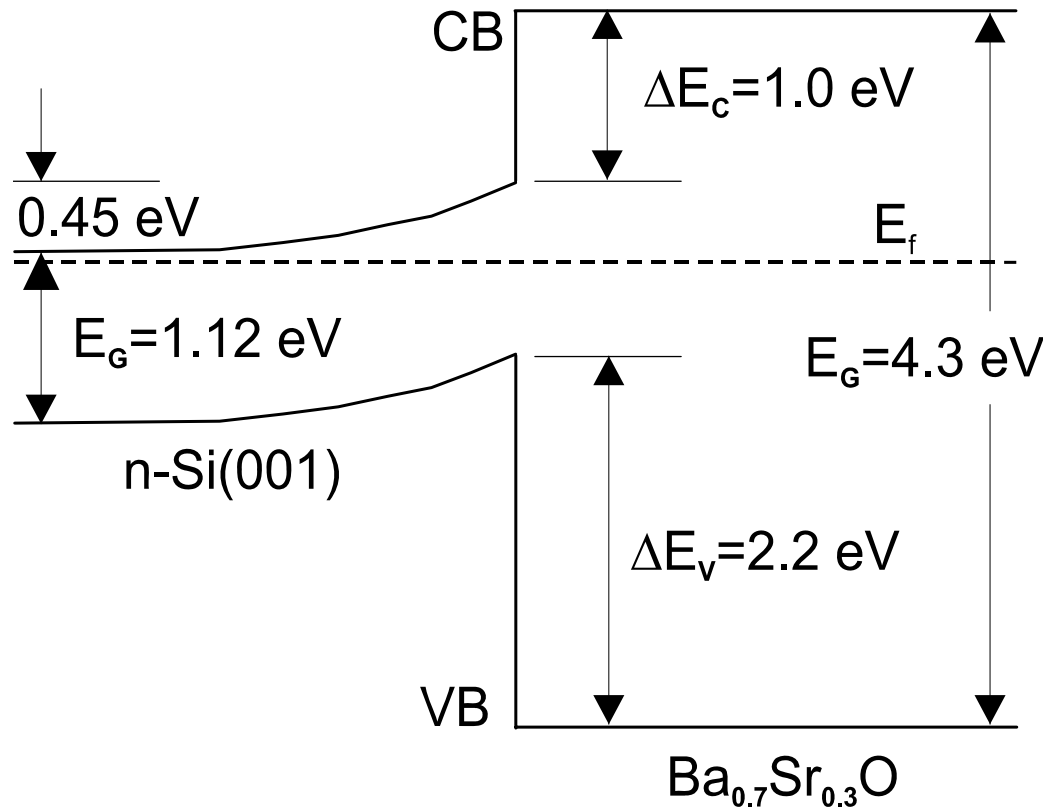
Independence of  $\text{Ba}_{0.7}\text{Sr}_{0.3}\text{O}$  band gap width on layer thickness



4.3 eV from 1 ML  $\rightarrow$  17 nm and more

# Electronic structure: Band gap and excitonic

Band alignment depending on the kind of interface



Intermediate layer 1.2 ML Sr

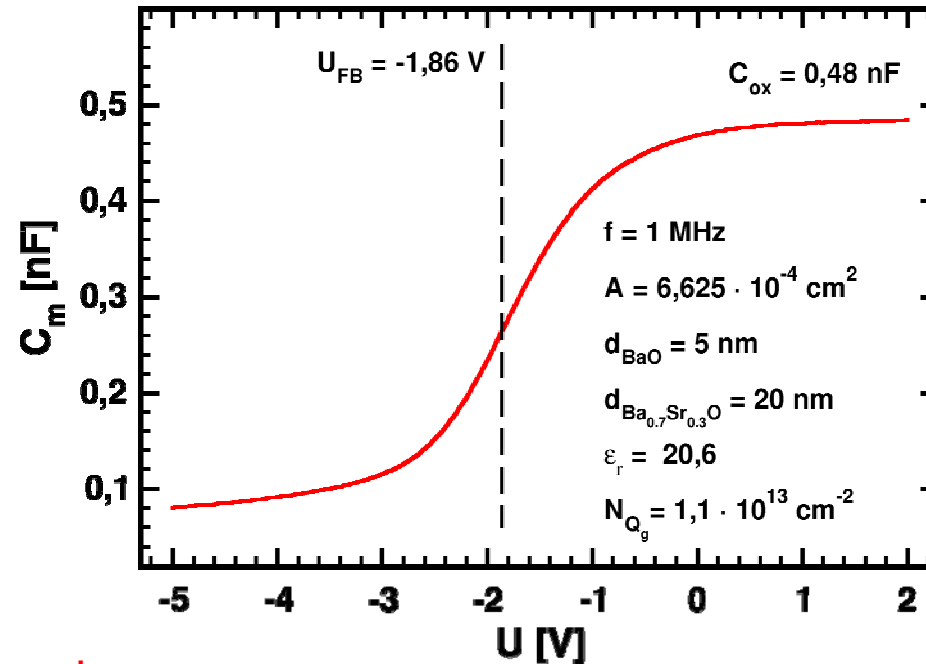
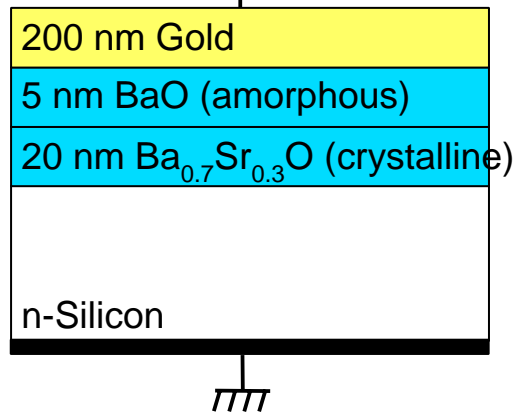
- band bending of n-Si(001) surface decreased by 0.09 eV
- but still depletion in silicon

$\Theta_I$	$\Delta E_v$	$\Delta E_c$
1.2 ML Sr	2.2	1.0
1 ML Sr	2.1	1.1
1 ML Ba	1.8	1.4

Tunable band alignment by different intermediate layer !

# Electrical characterization

## C-V- measurements



$\epsilon_r = 20,6$  from capacity at inversion

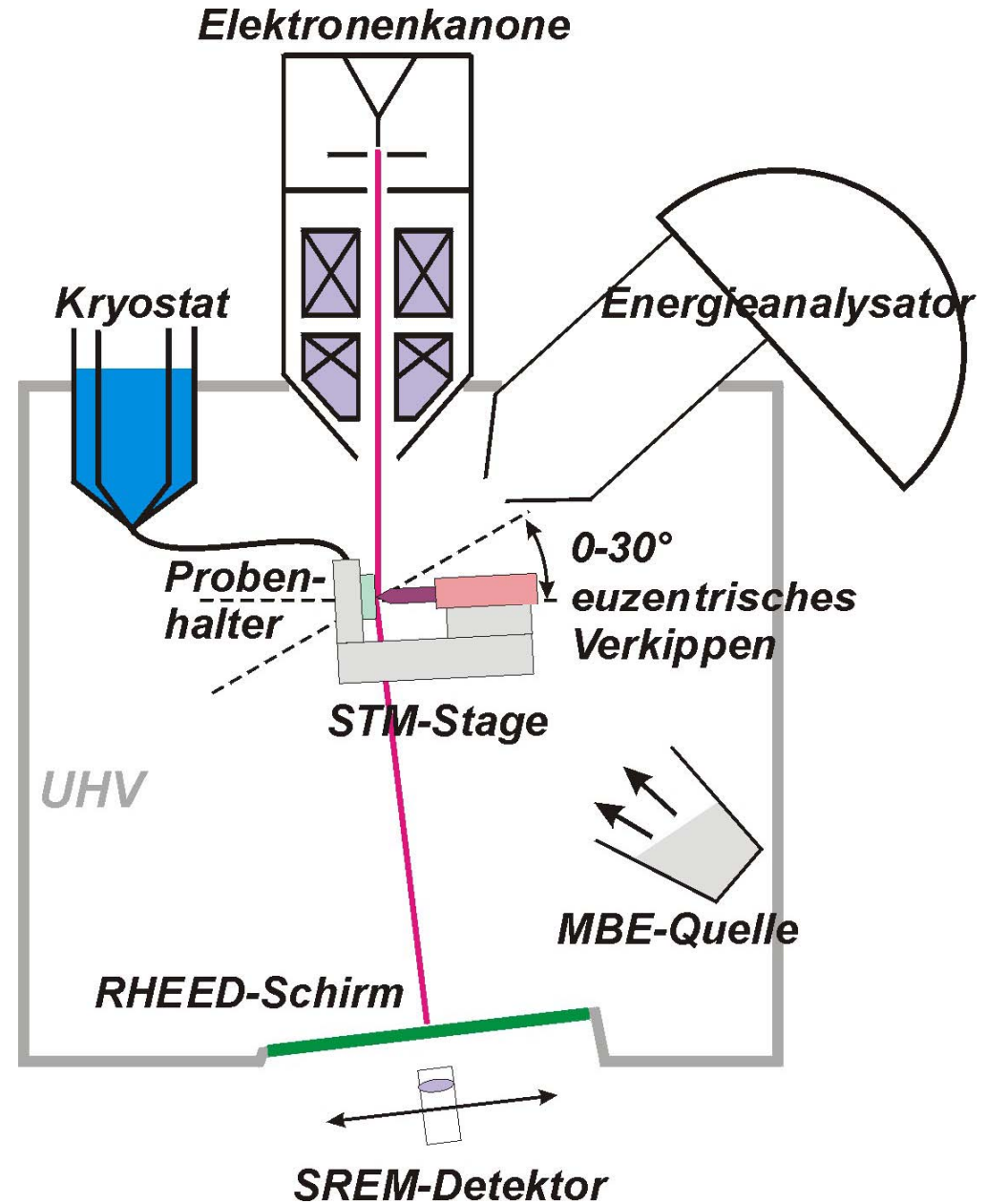
high charge density in oxide  $1,1 \cdot 10^{12} \text{ cm}^{-2}$

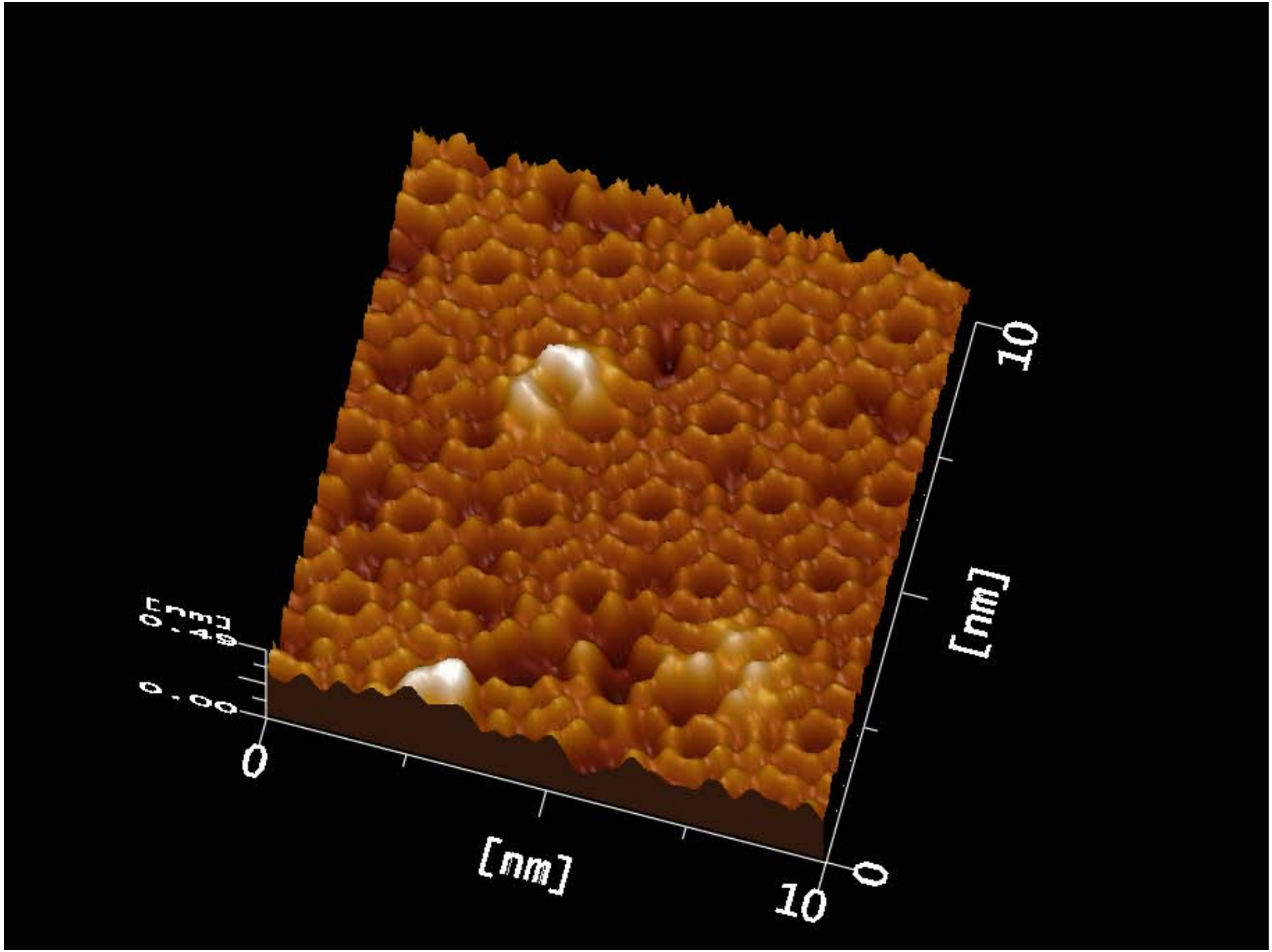
gradual increase → high surface state density  $D_{it}$

small hysteresis → low density of mobile charges in oxide

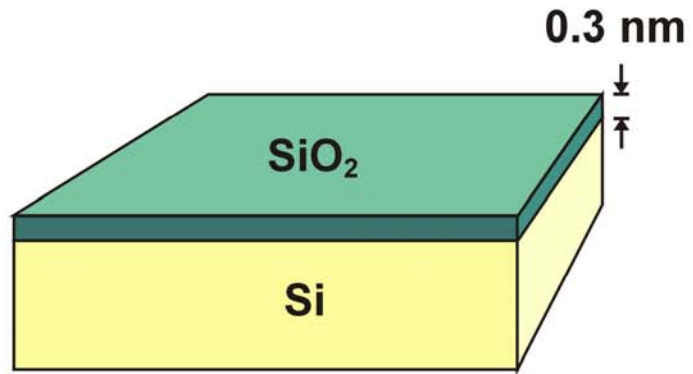


# Neuartige Strukturierungs- verfahren: SEM + STM im UHV

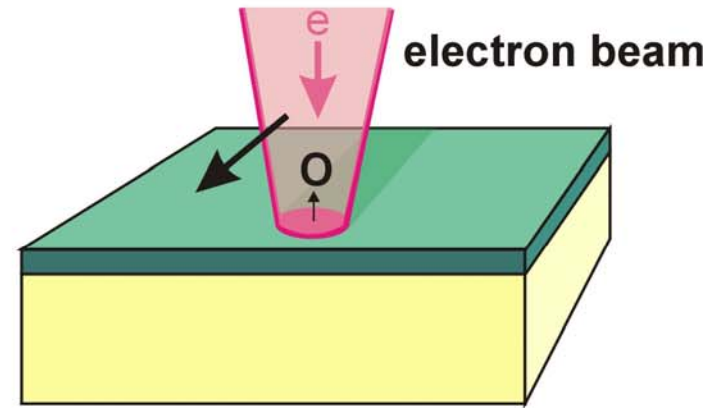




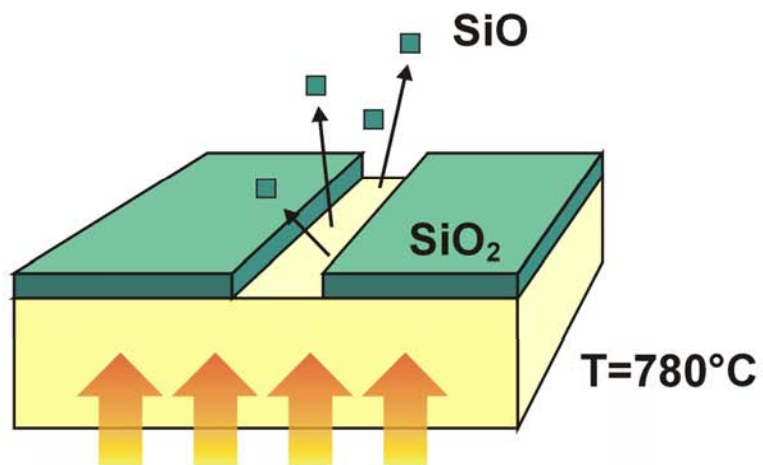
1)



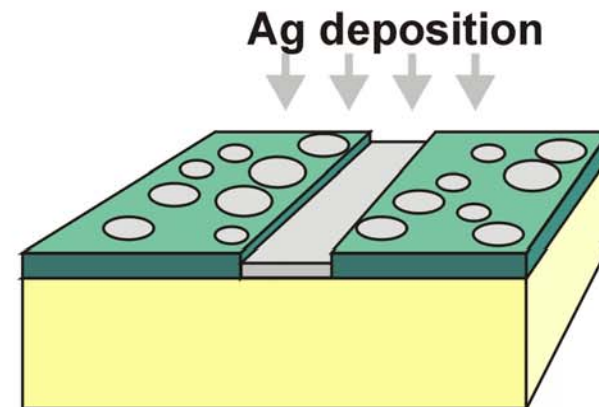
2)



3)

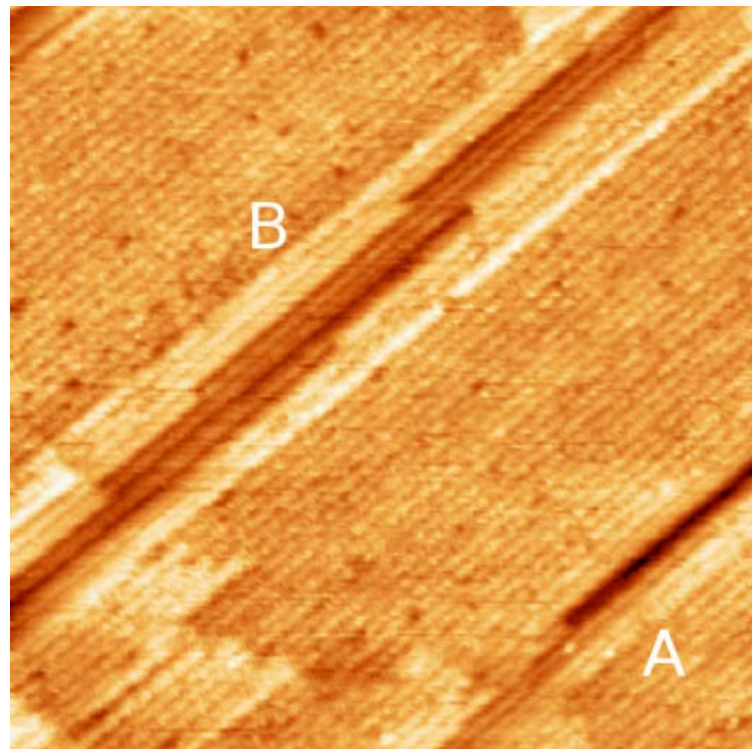


4)



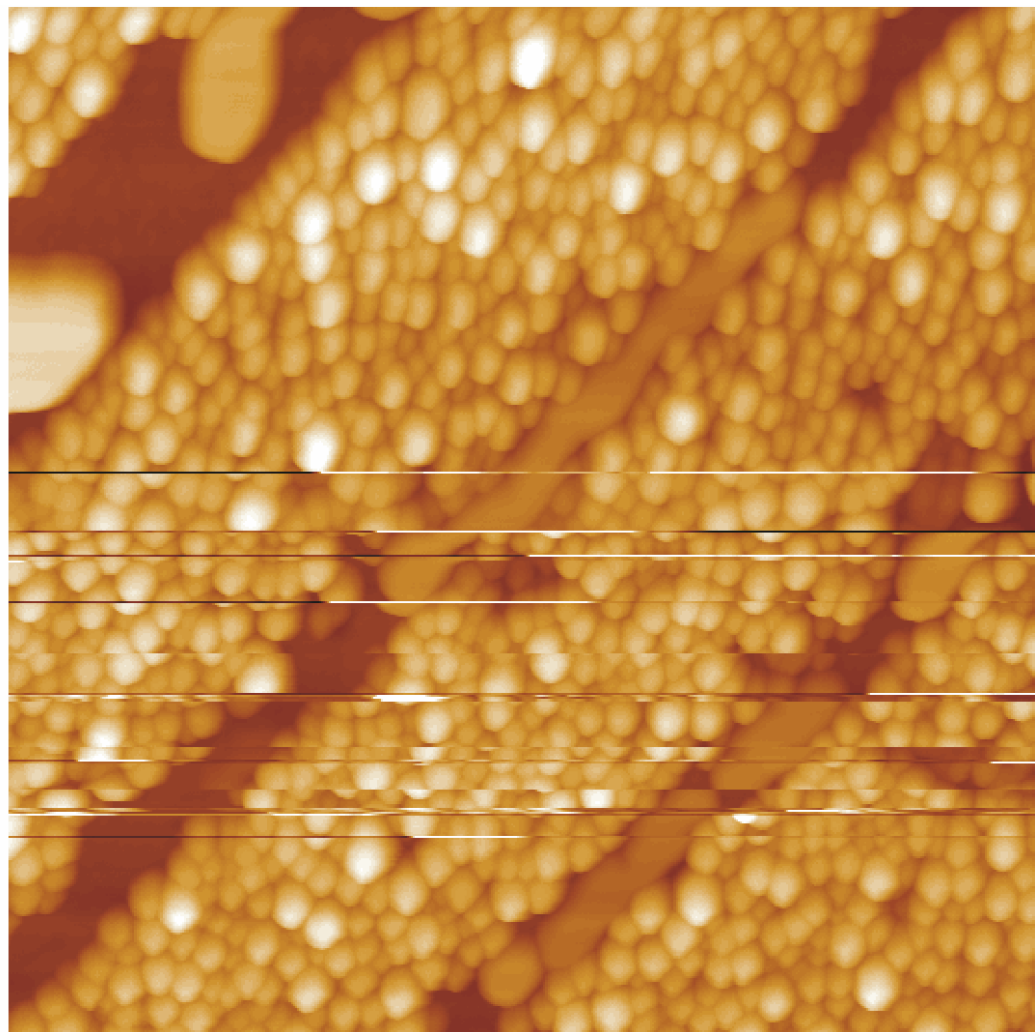
# Kombination mit gestufter Fläche

a)

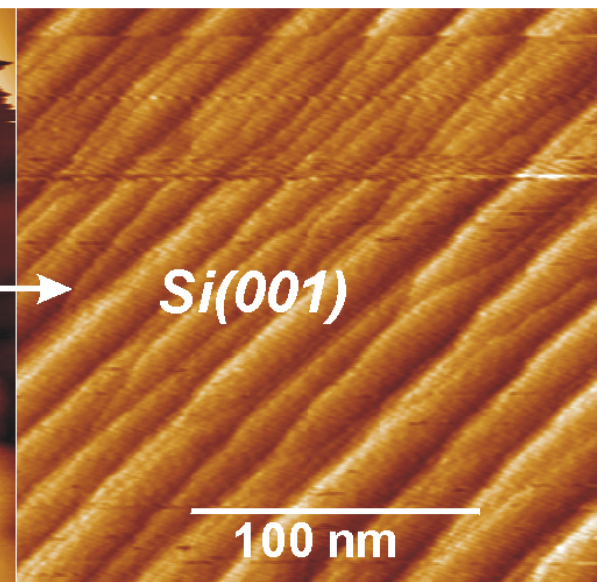
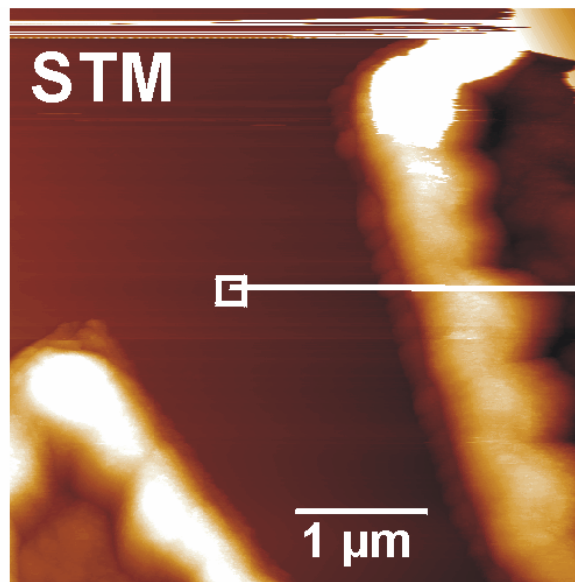
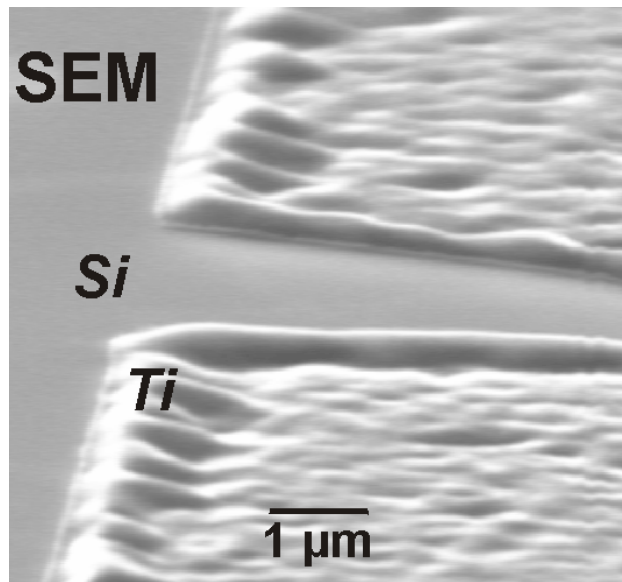


100 nm

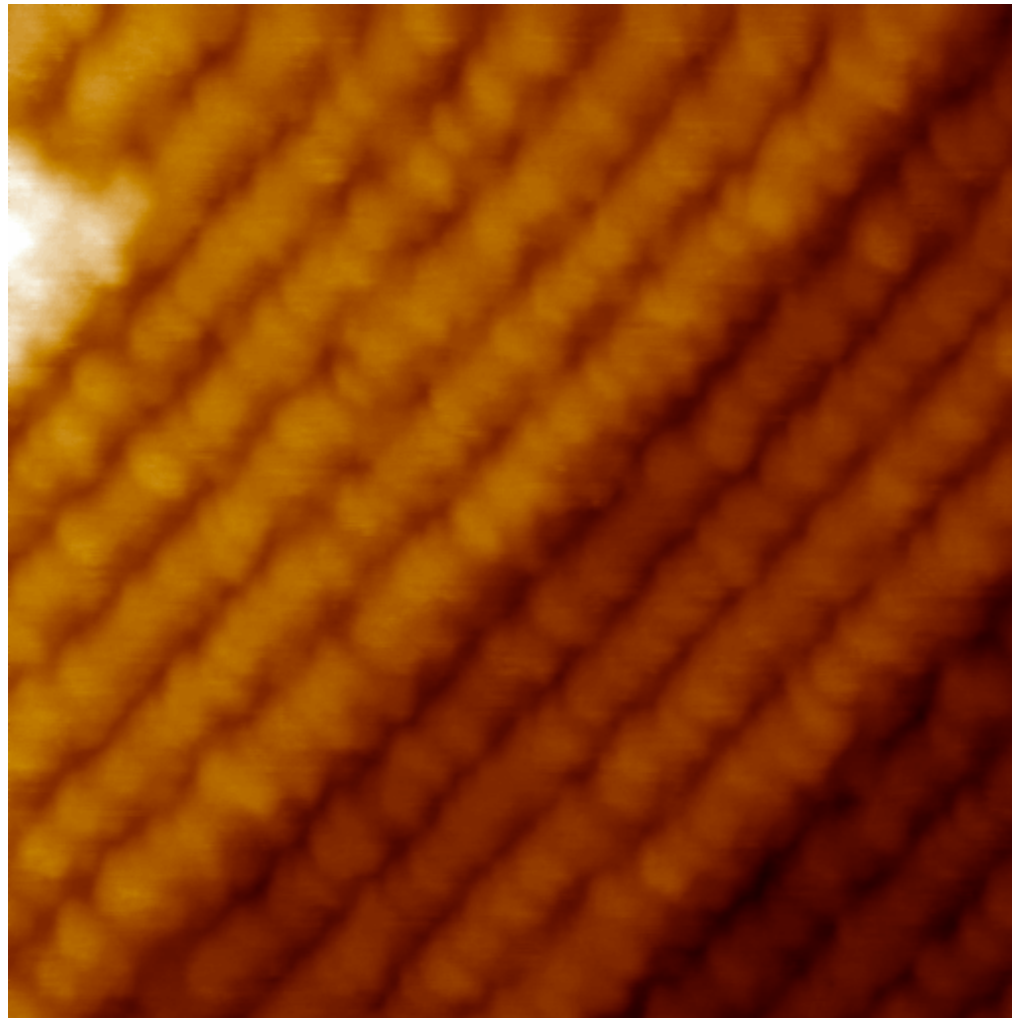
b)



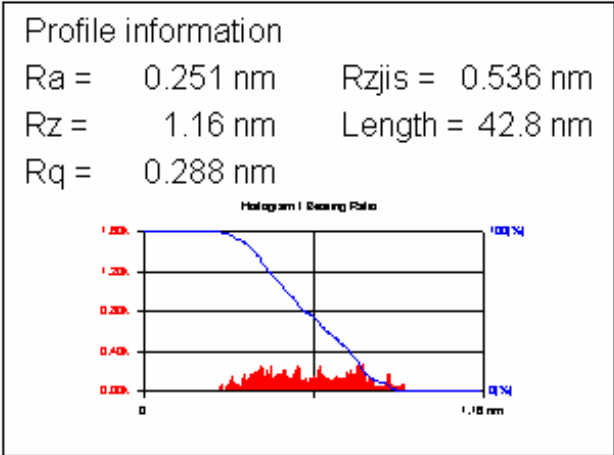
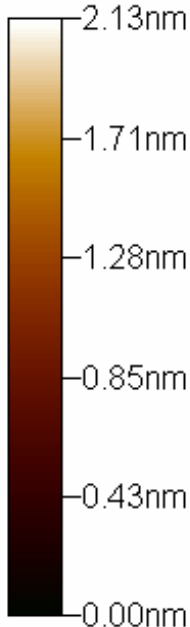
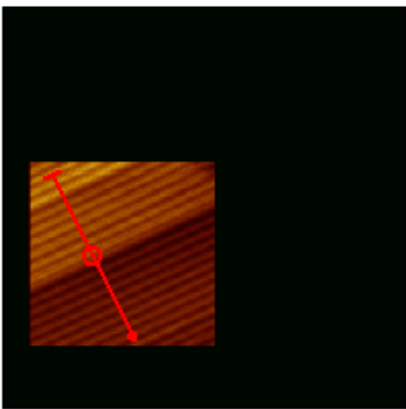
# TiSi contact pads



Kombination mit Selbstorganisation:  
Blei auf Si(557)

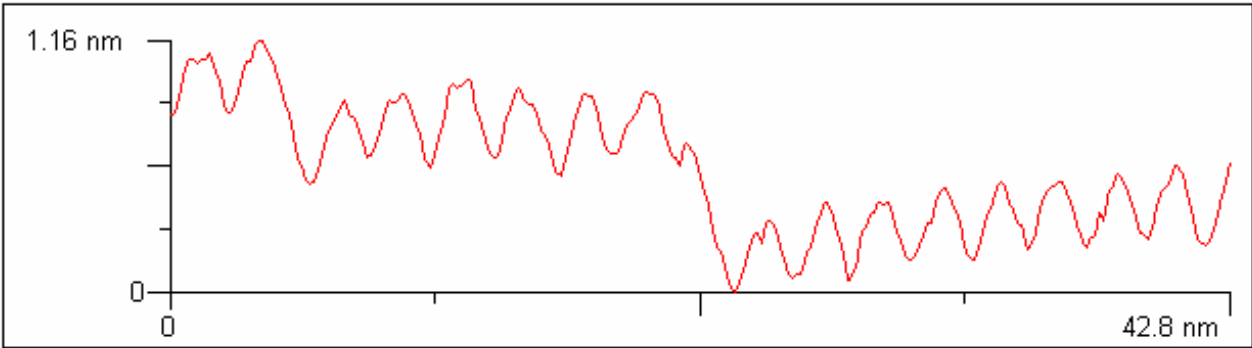


# Umordnung der Fläche durch Bleiadsorption

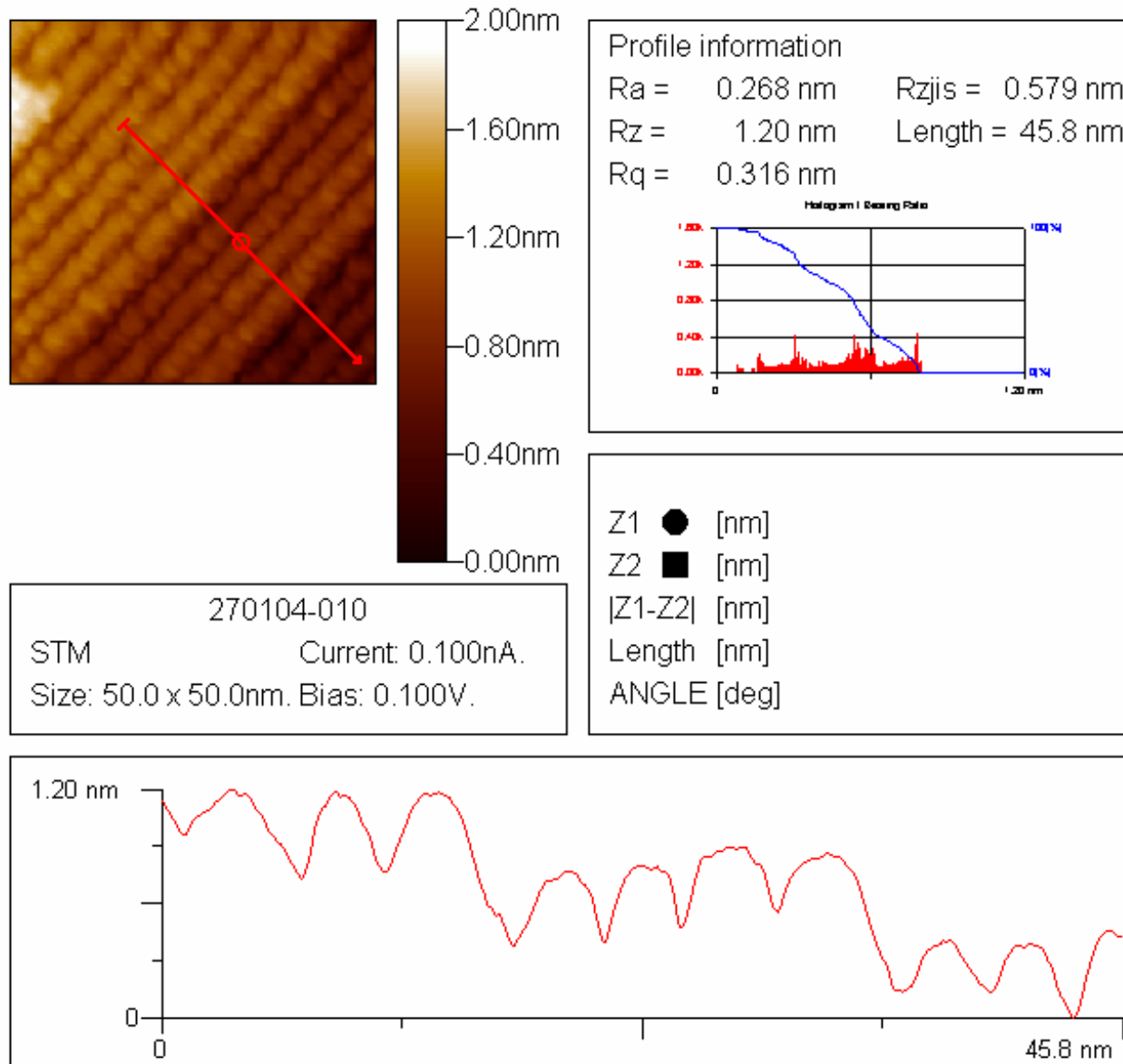


260104-001  
 STM                      Current: 0.200 nA.  
 Size: 92.9 x 92.9 nm. Bias: 2.000 V.

Z1 ● [nm]  
 Z2 ■ [nm]  
 |Z1-Z2| [nm]  
 Length [nm]  
 ANGLE [deg]



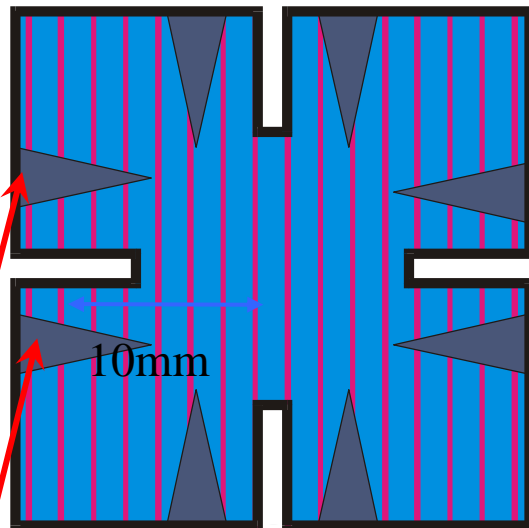
# Umordnung der Fläche durch Bleiadsorption





# Macroscopic dc measurement

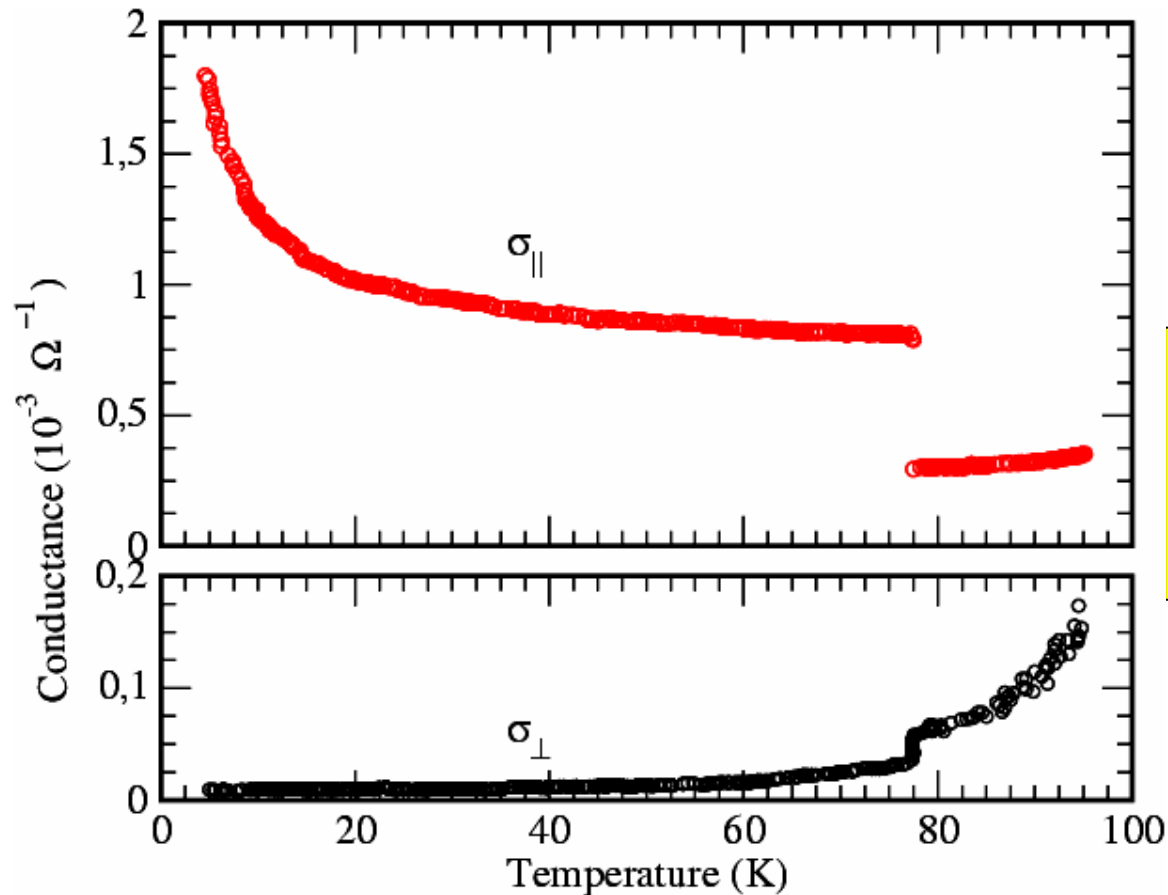
modified  
v.d.Pauw geometry



TiSi<sub>2</sub> contacts

Measurements  
parallel and  
perpendicular to  
step edges

# High temperature annealing (T= 640 K)



$\Theta \sim 1$  ML left

Phase transition at 78K:  
switching from small to  
large anisotropy

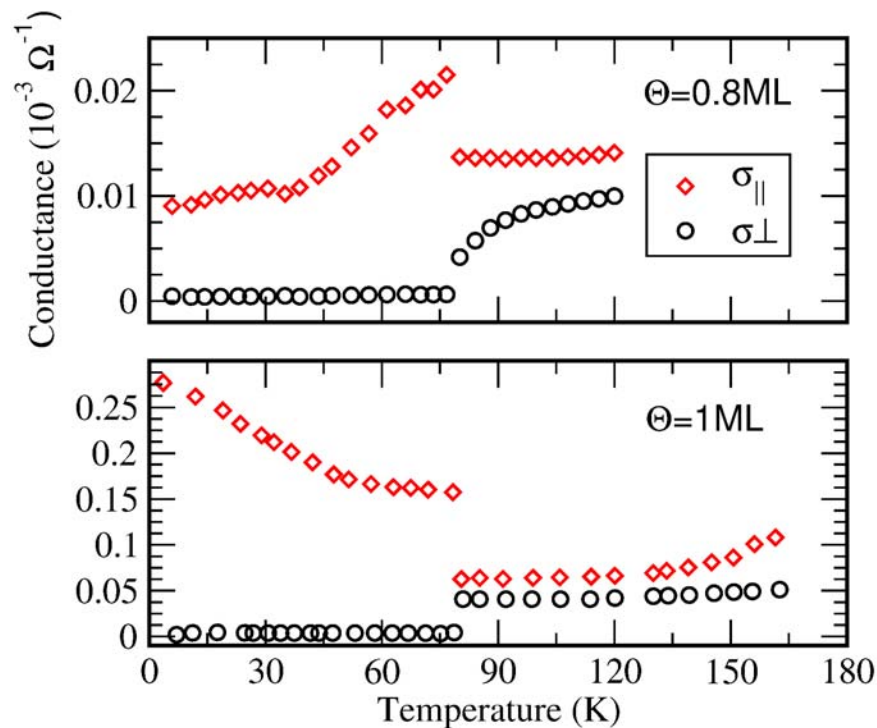
$\sigma_{\parallel}$  large:  
Conductance in surface  
state  
Defects unimportant

# Transport: Localization due to Fermi-nesting

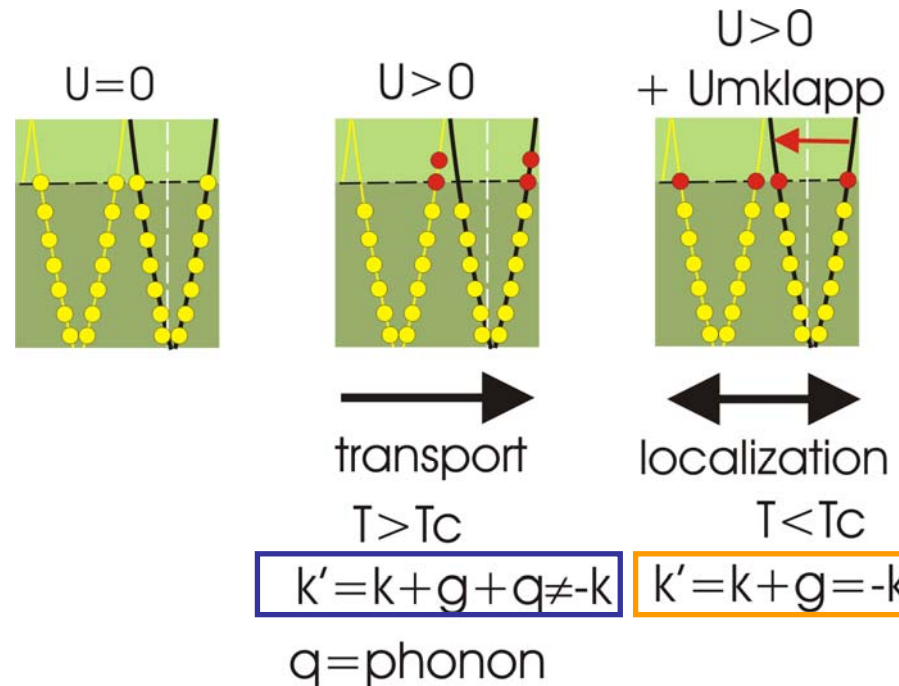
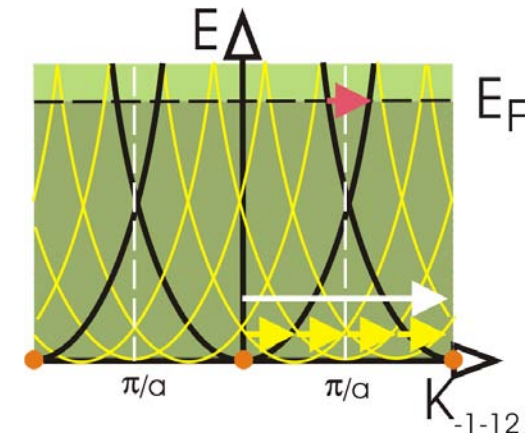
## Conductivity experiment:

$T < T_c$ :  
insulating across wires  
metallic along wires

## STM: order-disorder transition

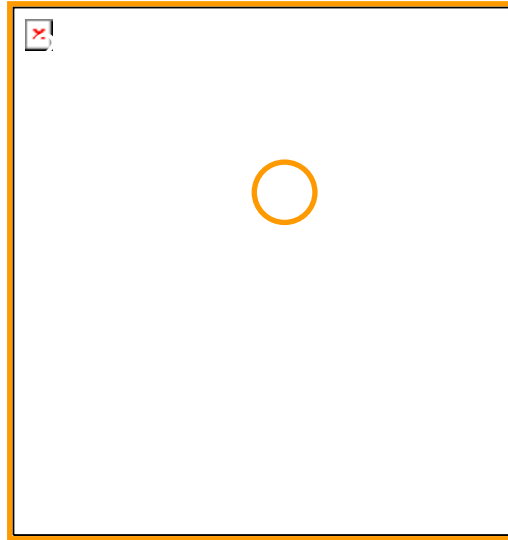


## Model:

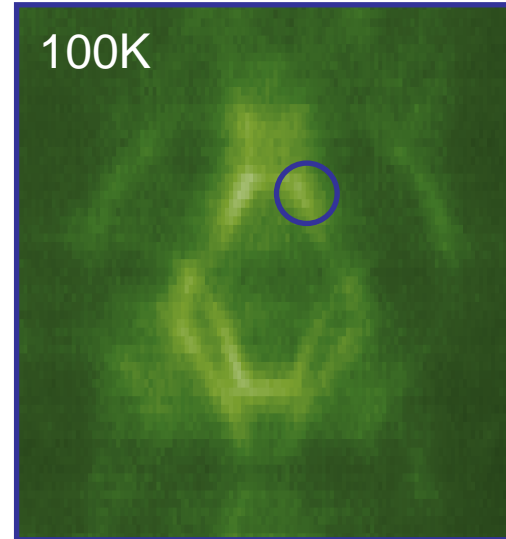


# Transition: Complete and incomplete Fermi-nesting

localization  
 $T < T_c$   
 $k' = k + g = -k$

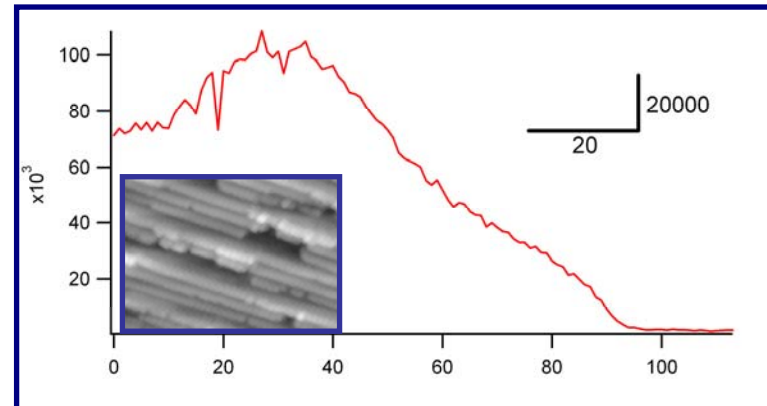
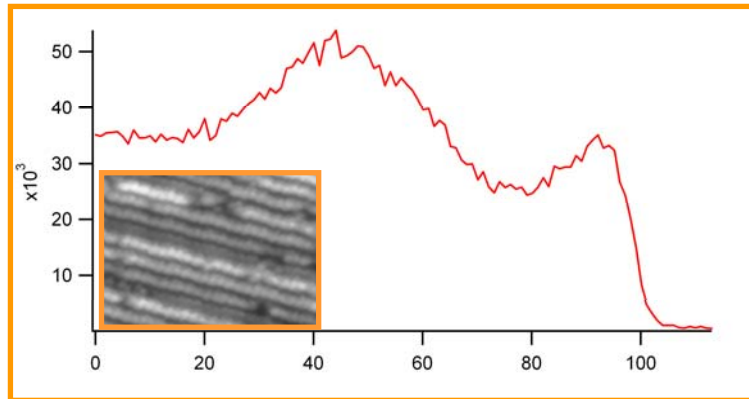


100K

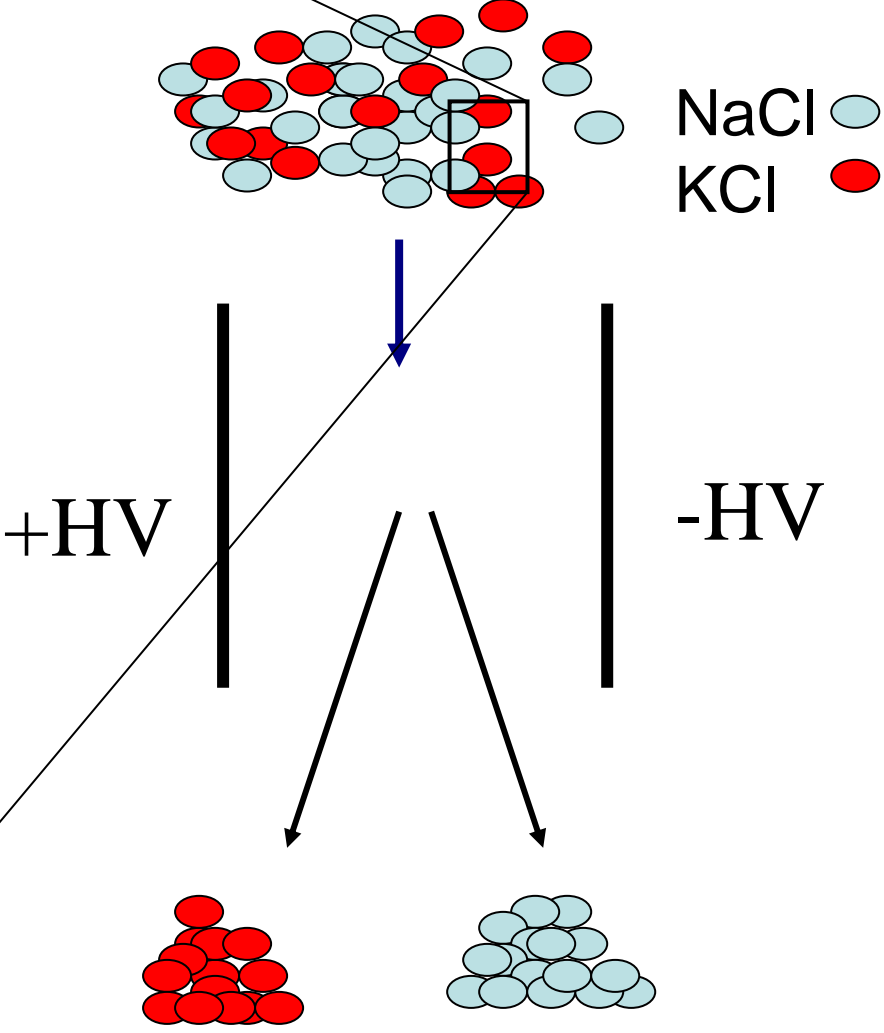
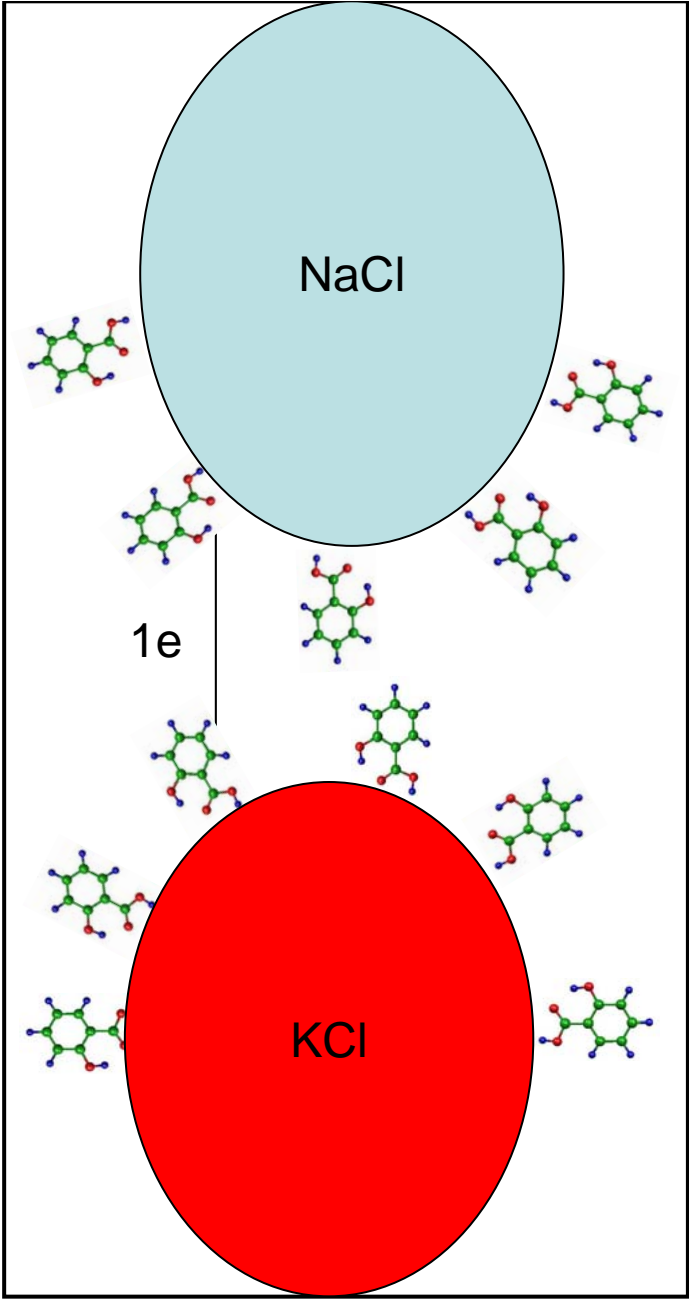


transport  
 $T > T_c$   
 $k' = k + g + q \neq -k$   
 $q = \text{phonon}$

Density of states

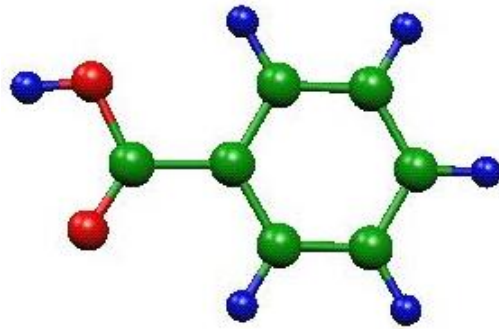


Ladungsübertrag von 1e notwendig  
in Gegenwart organischen Molekülen !!

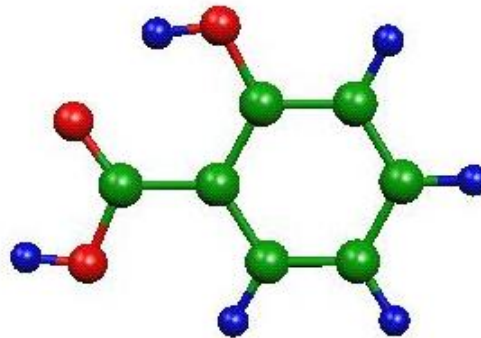
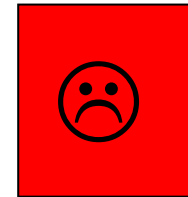
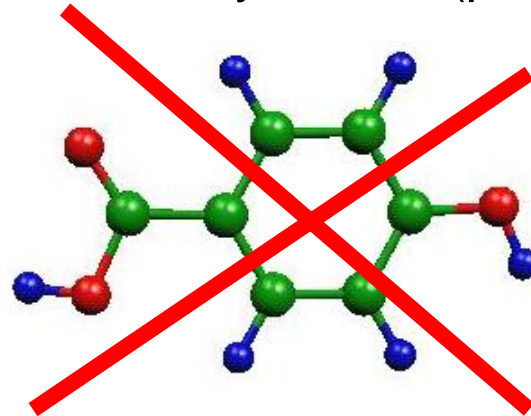


# Einfache organische Säuren als Konditionierungsmittel

Benzoessäure (BA)



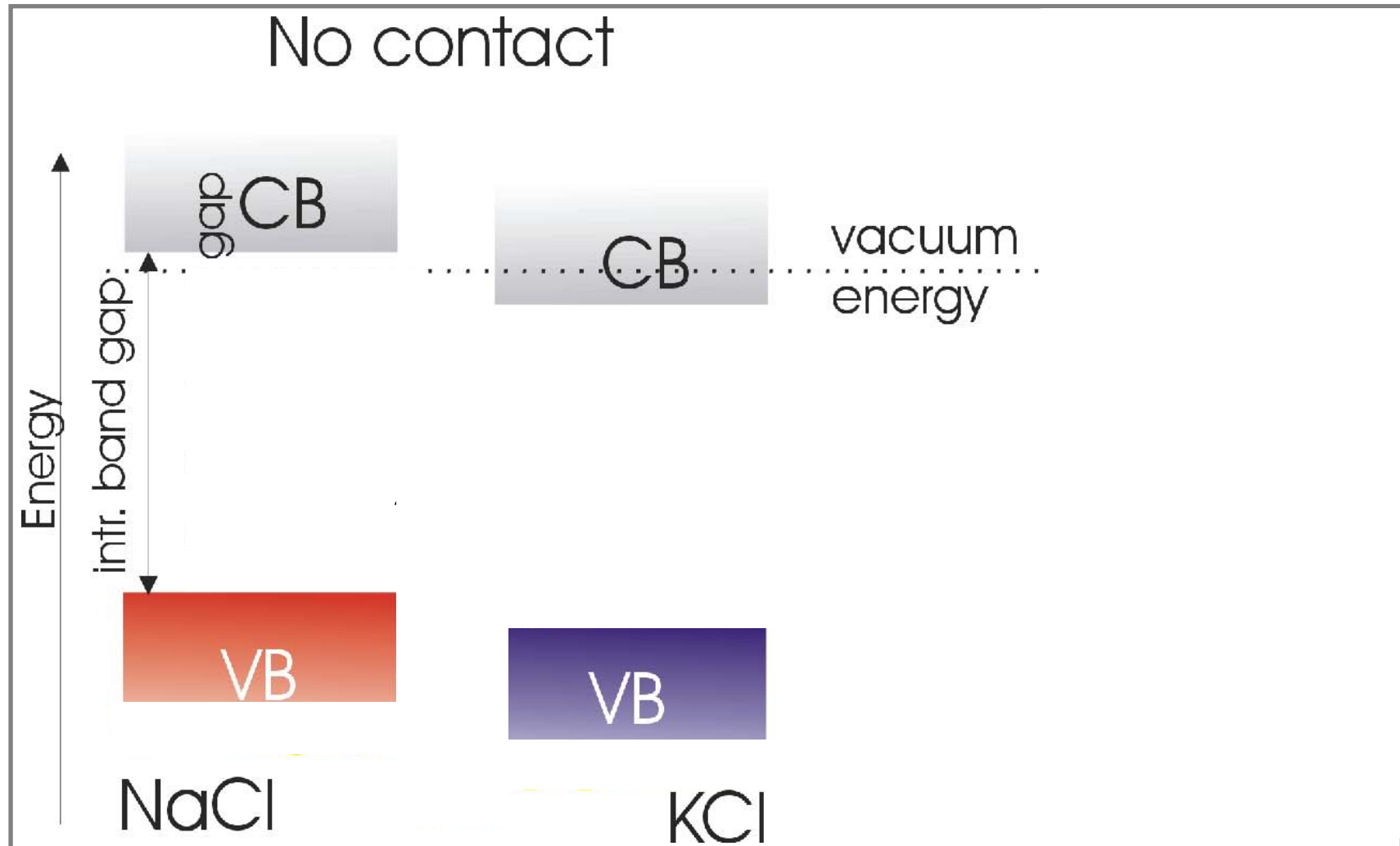
Para-Salicyl-Säure (p-SA)



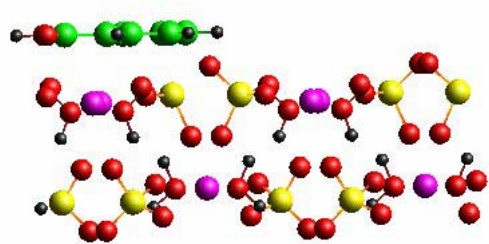
Salicyl-Säure (SA)

SA und p-SA:  
Gleiche chemische Zusammen-  
setzung !!

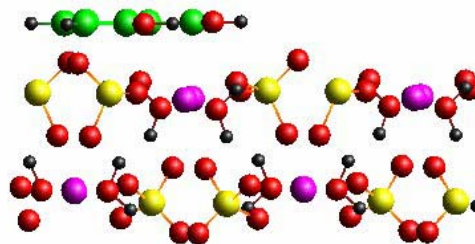
## Modell:



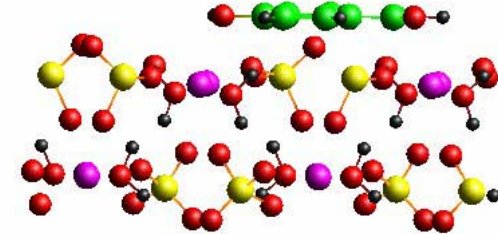
# MgSo4: Adsorptionsgeometrien für organische Säuren



benzoic acid



salicylic acid

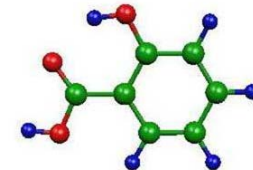


para-salicylic acid

Moleküle gedreht:

Quasi-aromatisches System von SA gestört!

Anderer Mechanismus der Kontaktaufladung:  
Obige Säuren inaktiv!





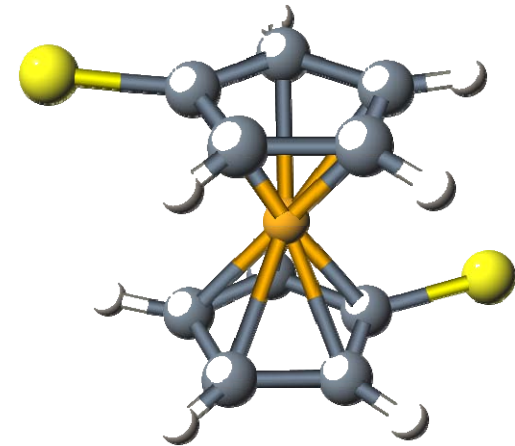
# Kontaktierung von Einzelmolekülen

## Ferrocen-dithiol

*Rotationsfreiheitgrad der Komplexbindung  
(Rechnung: 40meV)*

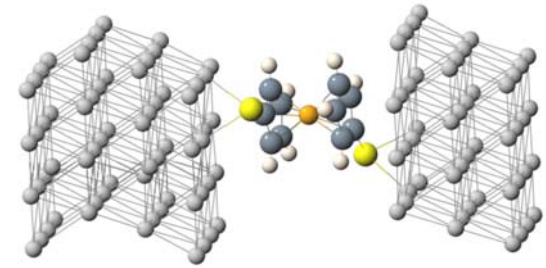
*Bindung zum Kontakt über SH,CN,.....*

*Hohe Leitfähigkeit*



**AG Butenschön**

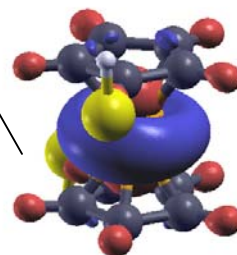
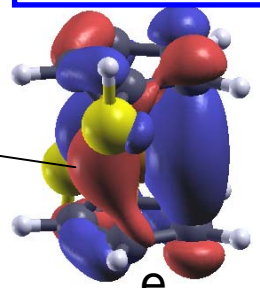
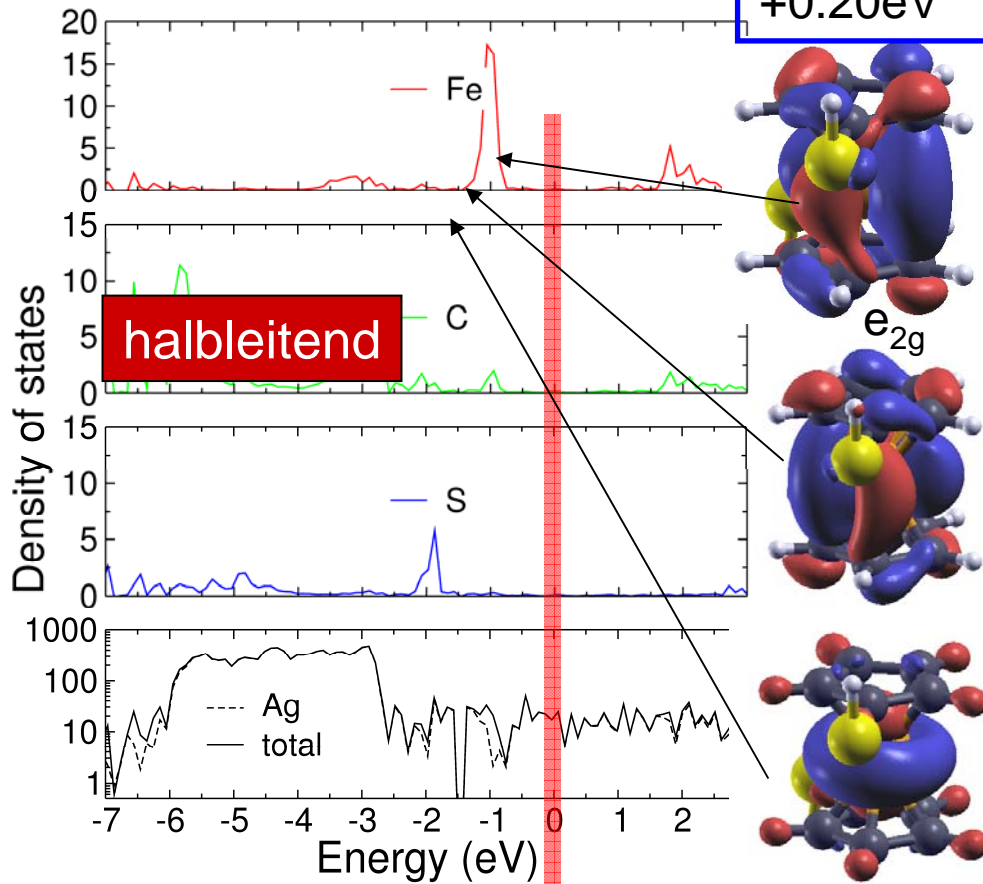
# FDT zwischen Ag(111) Kontakten



## Thiol gebunden (Ag-SH):

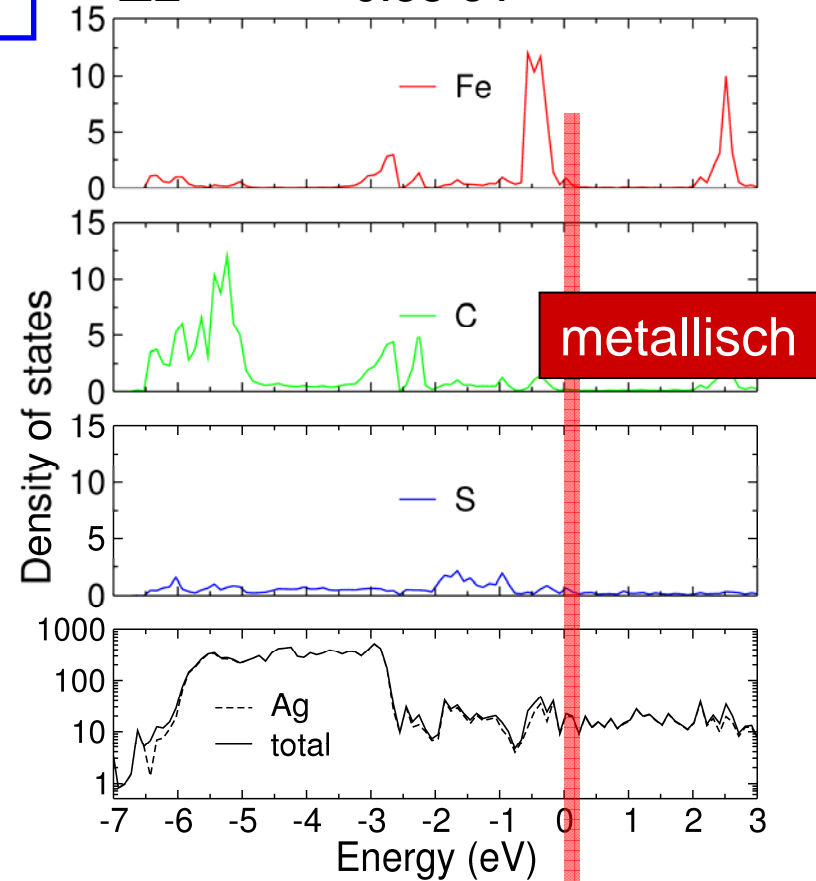
$$\Delta E^{\text{thiol}} = -0.30 \text{ eV}^*$$

$$\Delta E^{\text{thiolate+H}} = +0.20 \text{ eV}$$



## Thiolat gebunden (Ag-S):

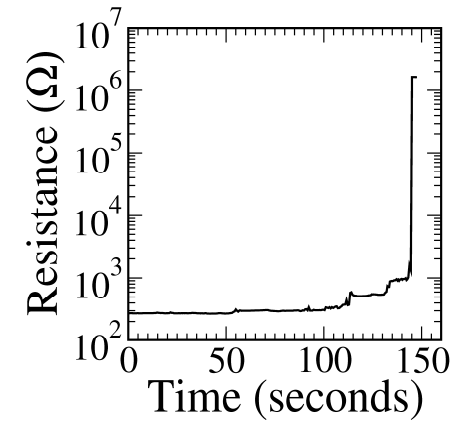
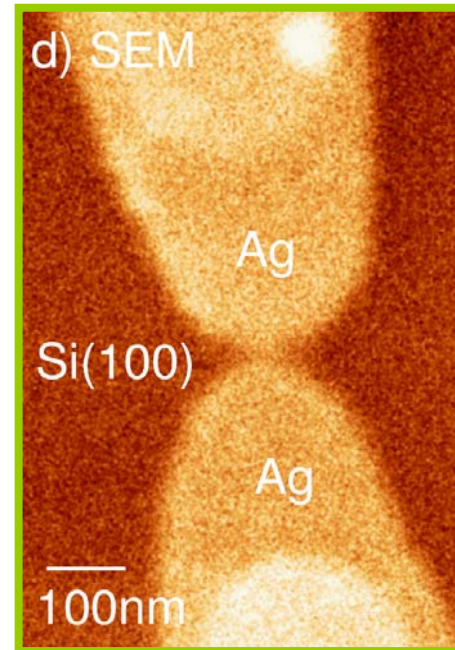
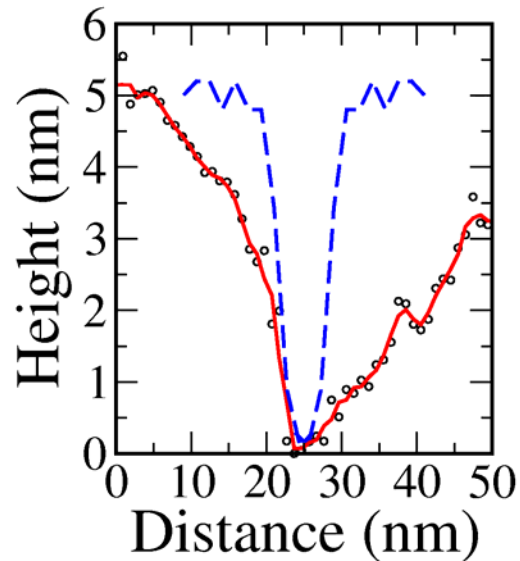
$$\Delta E^{\text{thiolate}} = -0.38 \text{ eV}^*$$



*J. Meyer, et.al. J. Chem. Phys. (2006).*

# Ultradünne Kontakte

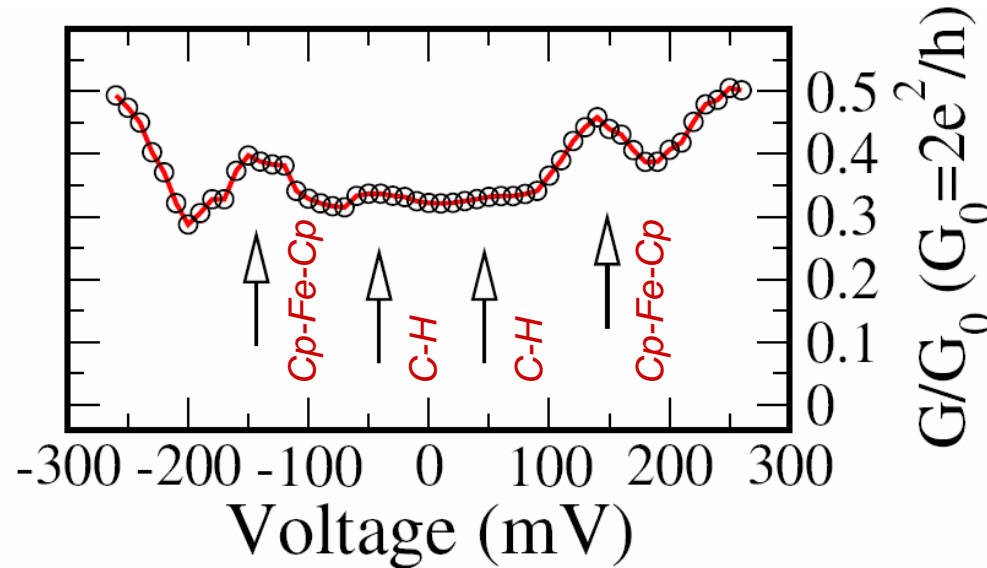
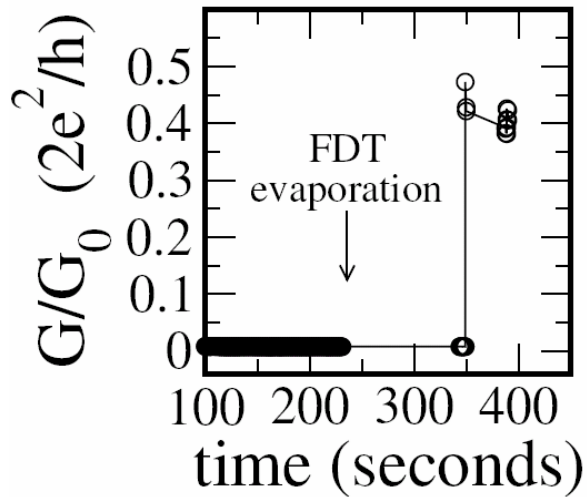
- Optimierte 3D Geometrie
- Herstellung über e-Lithographie
- Epitaktisches System Ag/Si(100)
- Öffnen: Elektromigration bei  $T=80\text{K}$
- Schließen des Kontaktes ( $T=300\text{K}$ )



Öffnen des Kontaktes  
Durch Elektromigration

**Lücke mit STM-Spitze zugänglich!**

# Leitfähigkeit eines FDT-Moleküls



## FDT induziert

- Kontakt offen:  $10^6$  Ohm  
Kontakt geschlossen:  $10^2$  Ohm

Leitfähigkeit:  $\sim 25 \mu A/V$  ( $0.35 G_0$ )

- $C_{11}$  :  $1.2 nA/V$  (exp.  $17 nA/V$ )  
OPE:  $1.7 \mu A/V$   
OPV:  $2.8 \mu A/V$

## Thiolat gebundene Systeme (metallic)

- Dissoziation an Defekten ?

## Sub-Struktur:

### Molekülresonanzen

### (spannungsinduzierte Übergänge)

(Ruitenbeek, PRL 2006)

Transport Rechnungen:

V. Maslyuk, AG I. Mertig, Uni Halle-Wittenberg

# Ausblick

- Grenzflächeneigenschaften zunehmend wichtiger
- Quantenbauelemente auch bei Raumtemperatur realisierbar
- Eingang in Alltags-Elektronik?
- Interdisziplinäres Arbeitsgebiet