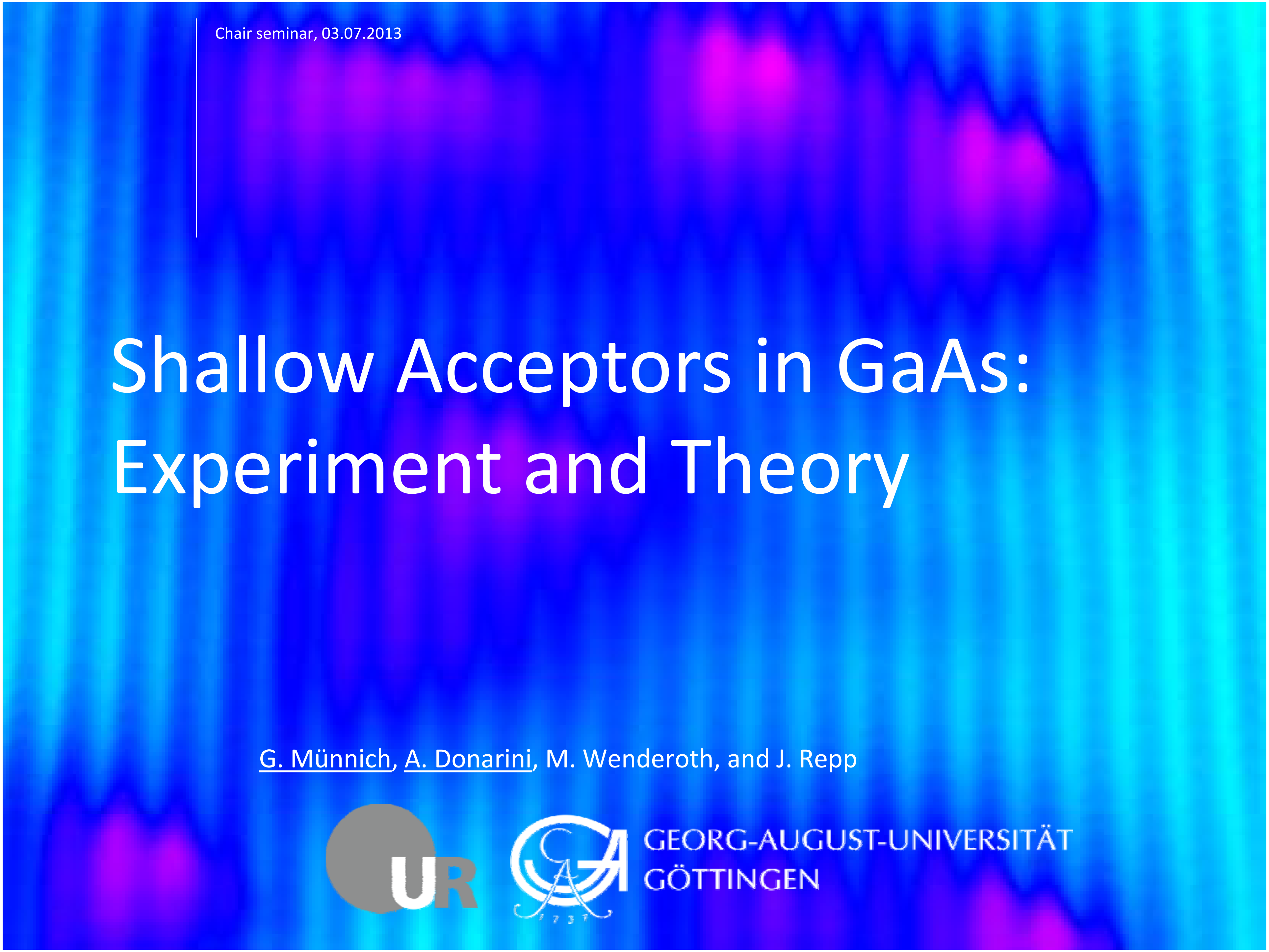


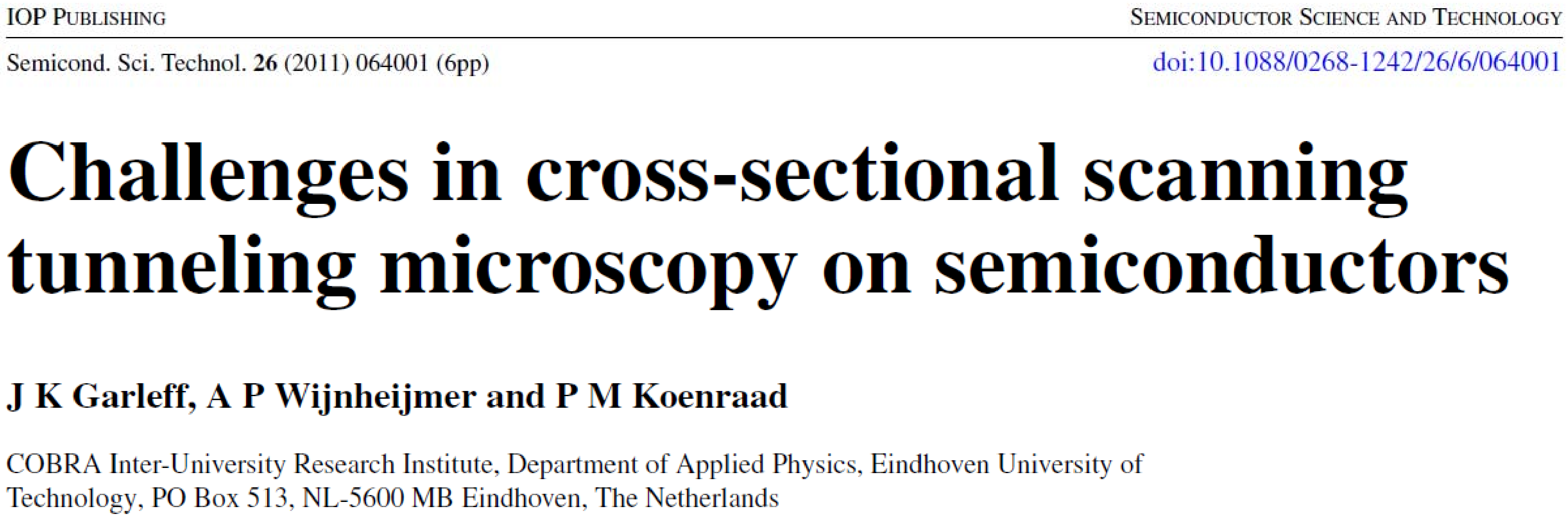
Chair seminar, 03.07.2013

Shallow Acceptors in GaAs: Experiment and Theory

G. Münnich, A. Donarini, M. Wenderoth, and J. Repp

UR

GEORG-AUGUST-UNIVERSITÄT
GÖTTINGEN



IOP PUBLISHING SEMICONDUCTOR SCIENCE AND TECHNOLOGY

Semicond. Sci. Technol. **26** (2011) 064001 (6pp) doi:10.1088/0268-1242/26/6/064001

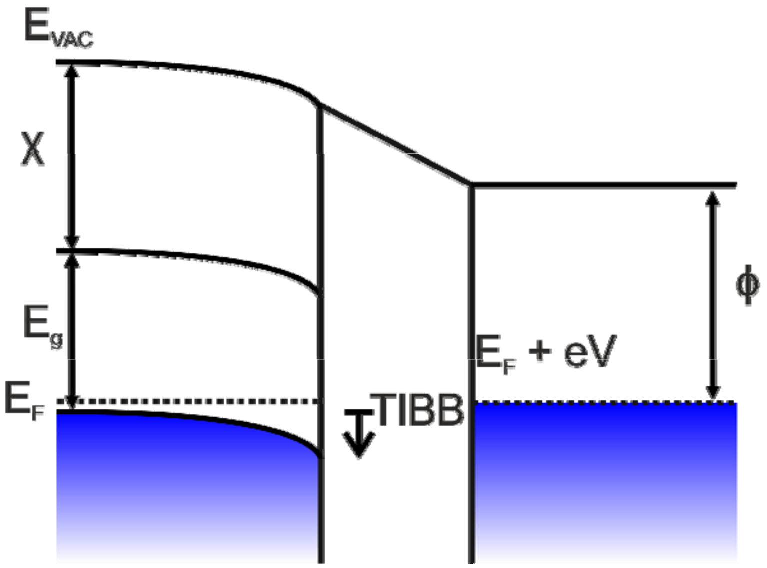
Challenges in cross-sectional scanning tunneling microscopy on semiconductors

J K Garleff, A P Wijnheijmer and P M Koenraad

COBRA Inter-University Research Institute, Department of Applied Physics, Eindhoven University of Technology, PO Box 513, NL-5600 MB Eindhoven, The Netherlands

1. Cleavage
2. Surface properties affecting impurities
3. Tip impact - TIBB

Tip induced band bending (TIBB)



- Unpinned Fermi-level:
  Applied bias voltage penetrates into sample
  -> tip induced band bending TIBB(V)

- TIBB(V) shifts the electronic position of all states below the tip

J. Vac. Sci. Technol. B **5**, 923 (1987)

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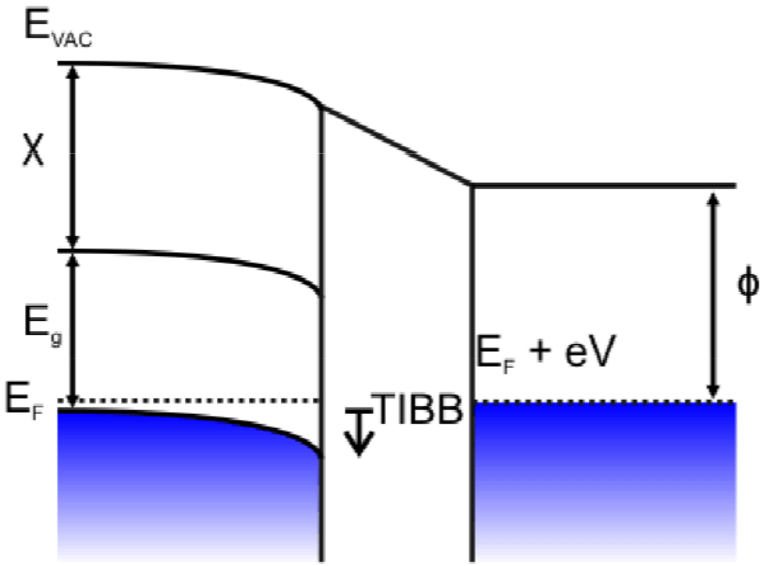

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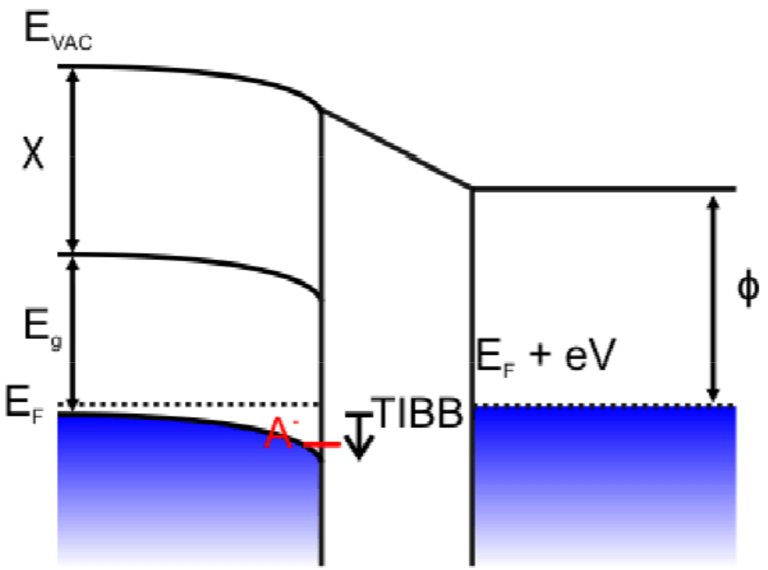

- Unpinned Fermi-level:
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  -> tip induced band bending TIBB(V)
- TIBB(V) shifts the electronic position of all states below the tip
- Electronic state can be shifted across the Fermi-level: Change of occupation $A^{-/0}$, change of contribution to tunneling

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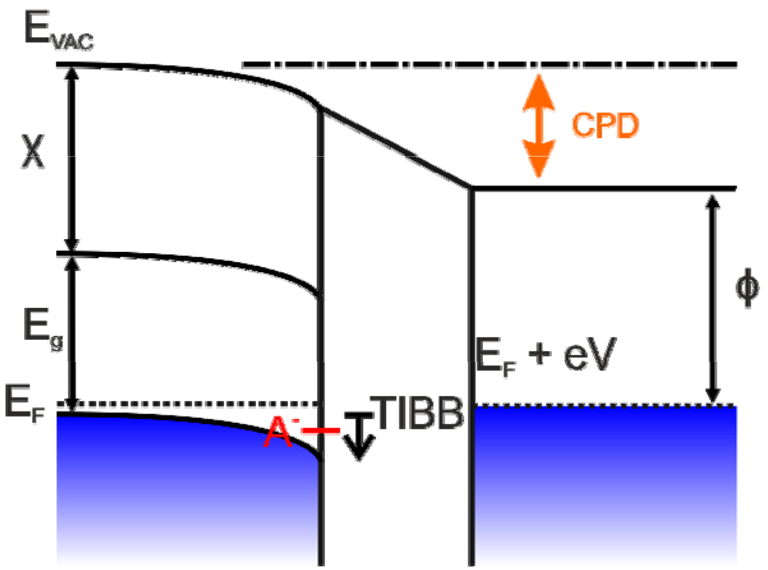

TIBB(V) can be negative for positive V, and
TIBB(V = ΔCPD/e) = 0

- Unpinned Fermi-level:
  Applied bias voltage penetrates into sample
  -> tip induced band bending TIBB(V)
- TIBB(V) shifts the electronic position of all states below the tip
- Electronic state can be shifted across the Fermi-level: Change of occupation $A^{-/0}$, change of contribution to tunneling
- TIBB(V) is non-zero even for zero bias, due to the contact potential difference ΔCPD between tip and sample

J. Vac. Sci. Technol. B **5**, 923 (1987)

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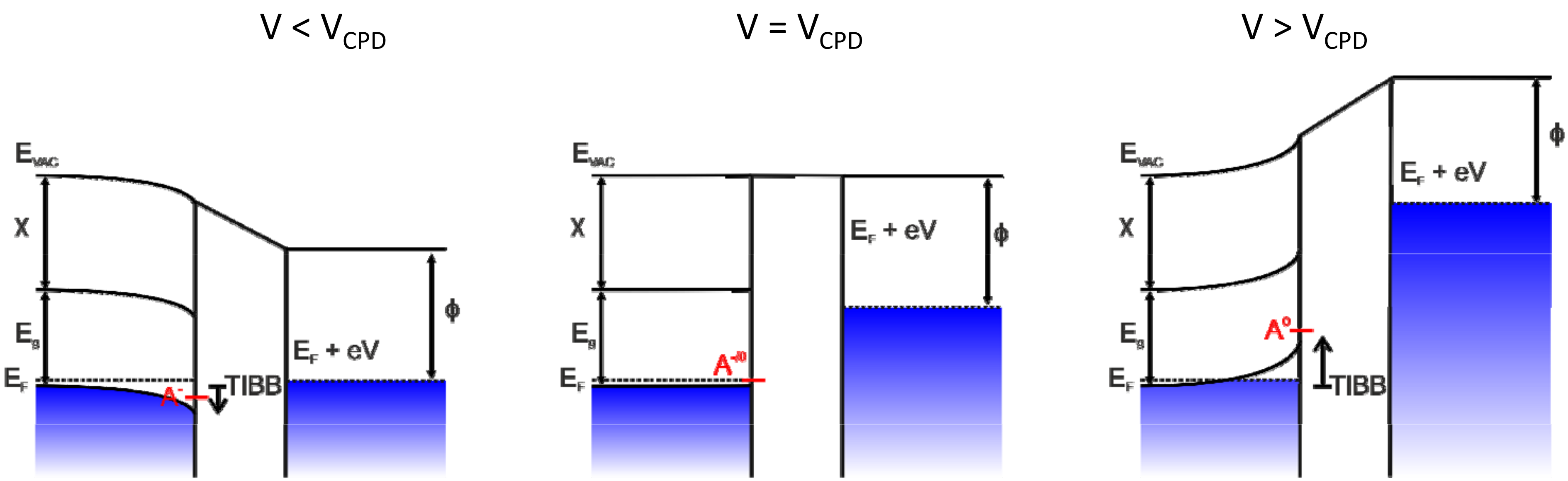
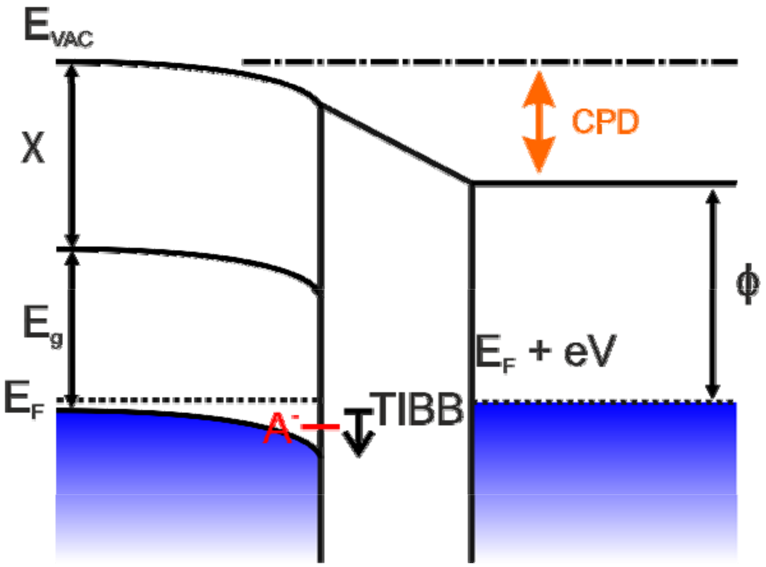


$V < V_{CPD}$ $V = V_{CPD}$ $V > V_{CPD}$

- If applied bias voltage cancels difference in work function between tip and sample, the bands are flat: TIBB($V = CPD/e = V_{CPD}$) = 0; State is at the Fermi level
- $V < V_{CPD}$: State is located below the Fermi level
- $V > V_{CPD}$: State is located above the Fermi level

Tip induced band bending (TIBB)



In STM, CPD and thereby the spectral position and charge state of electronic states is unknown

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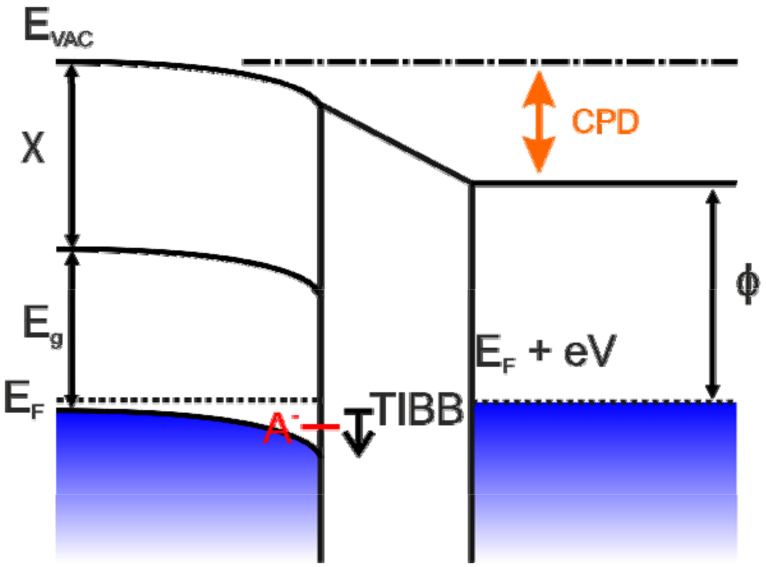
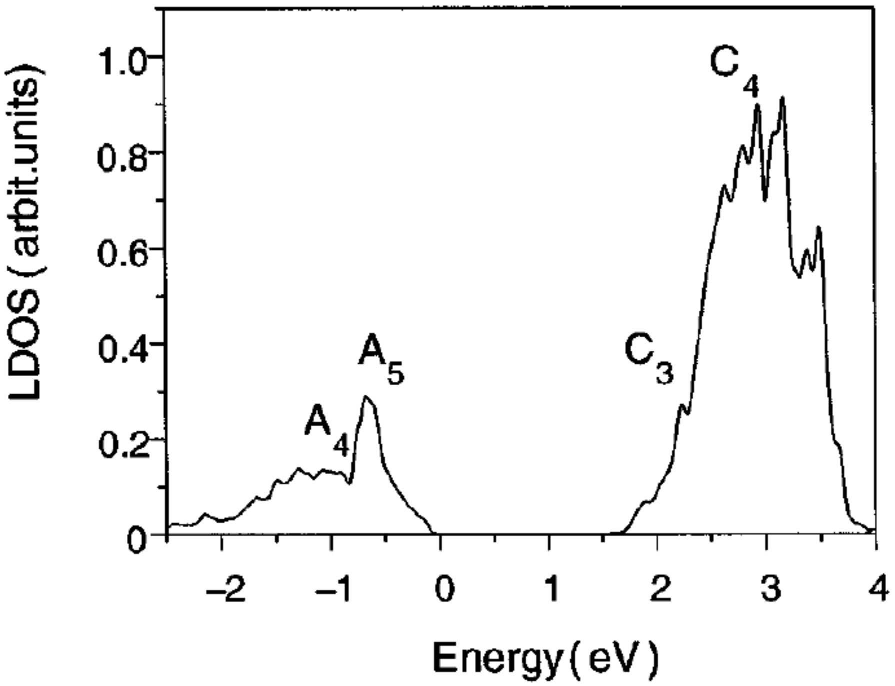


In STM, ΔCPD and thereby the spectral position and charge state of electronic states is unknown

Use combined STS/KPFM to relate spectroscopic data to the flat-band voltage

Electronic properties the GaAs(110) surface

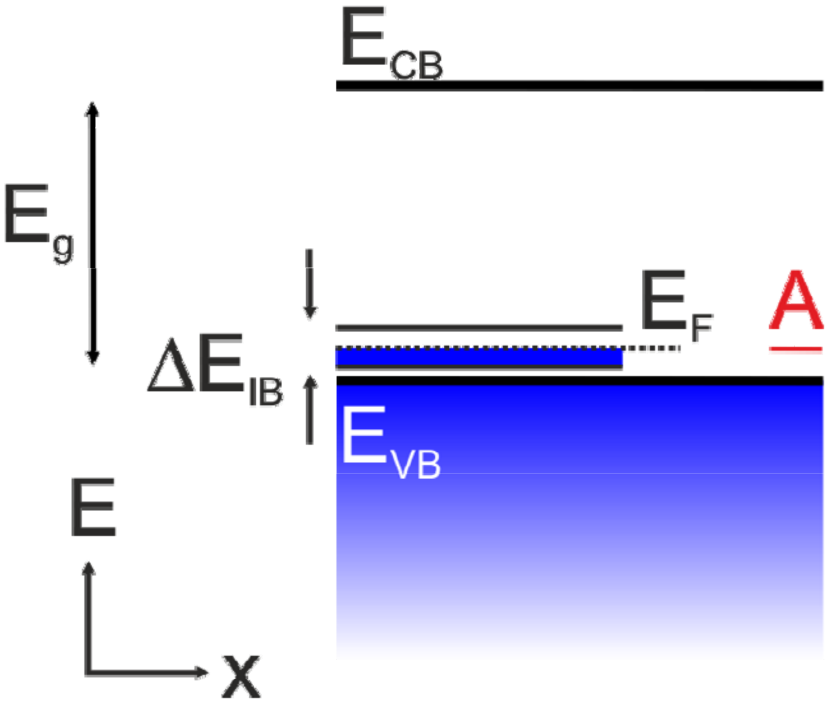


- 4 surface resonances outside the band gap

- Fermi-level not pinned:
  -> tunneling is only possible for certain bias voltages
  -> bulk DOS is not masked

calculated DOS: Phys. Rev. Lett. **77**, 2997 (1995)

Electronic properties of Zn doped GaAs



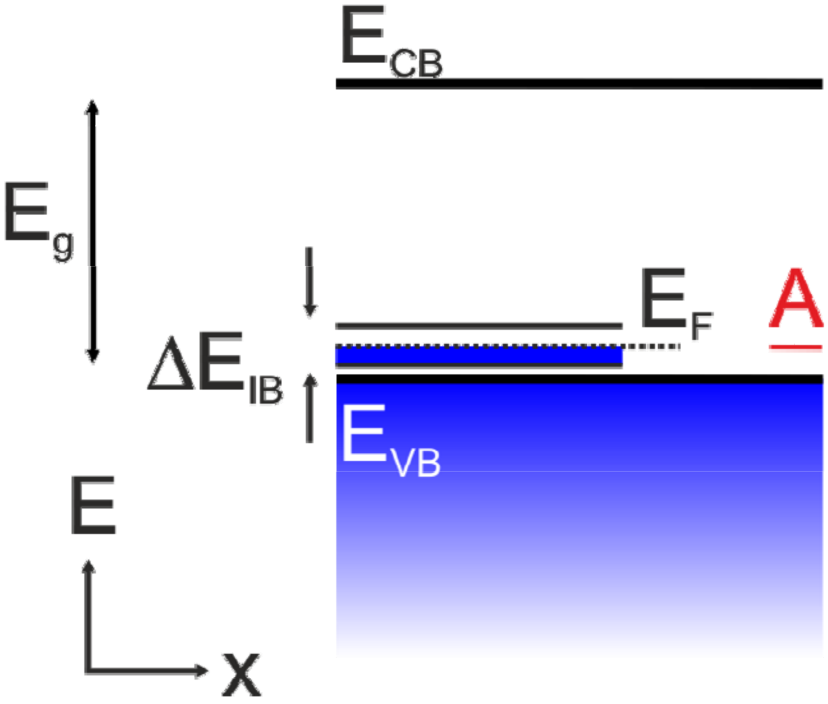
- Zn is an acceptor in GaAs
  -> p-type doping

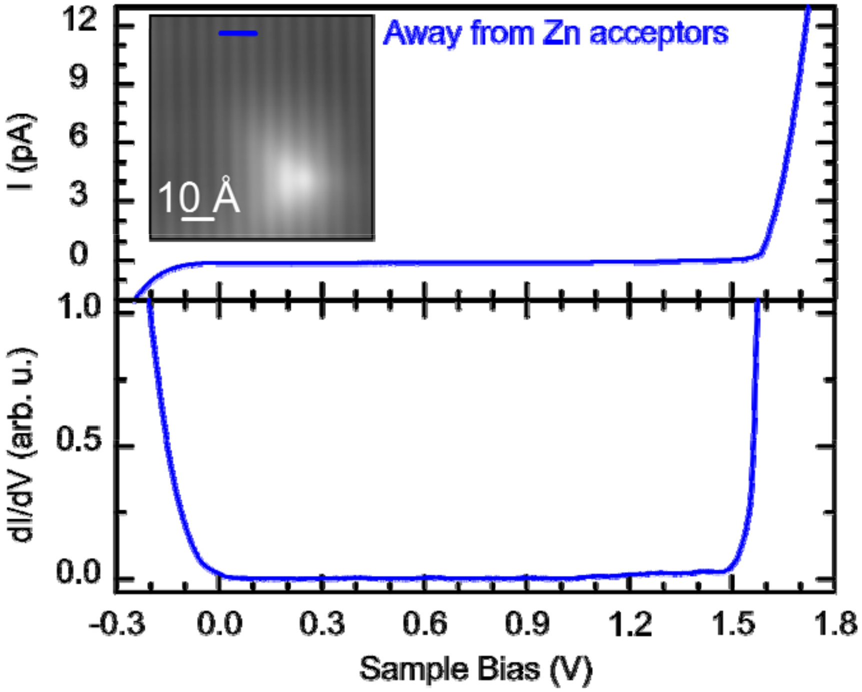
- Zn ionization energy in GaAs: 31 meV

- For the dopant concentration $1 \cdot 10^{19}$ Zn/cm^3 used here impurity band of ΔE_{IB} = 24 meV width is established

E. F. Schubert: Doping in III-V Semiconductors,
Cambridge University Press, 1993

Electronic properties of Zn doped GaAs





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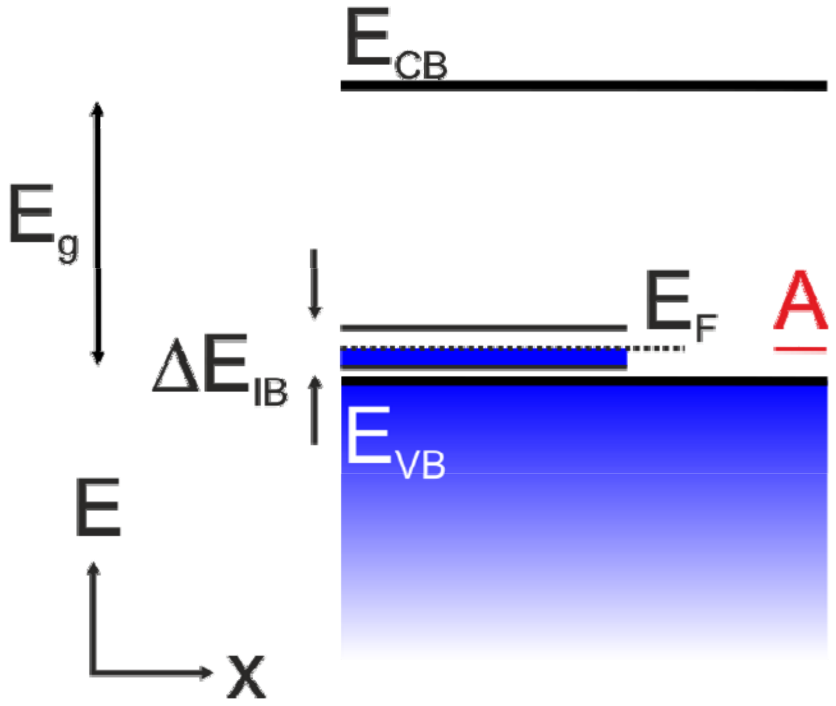
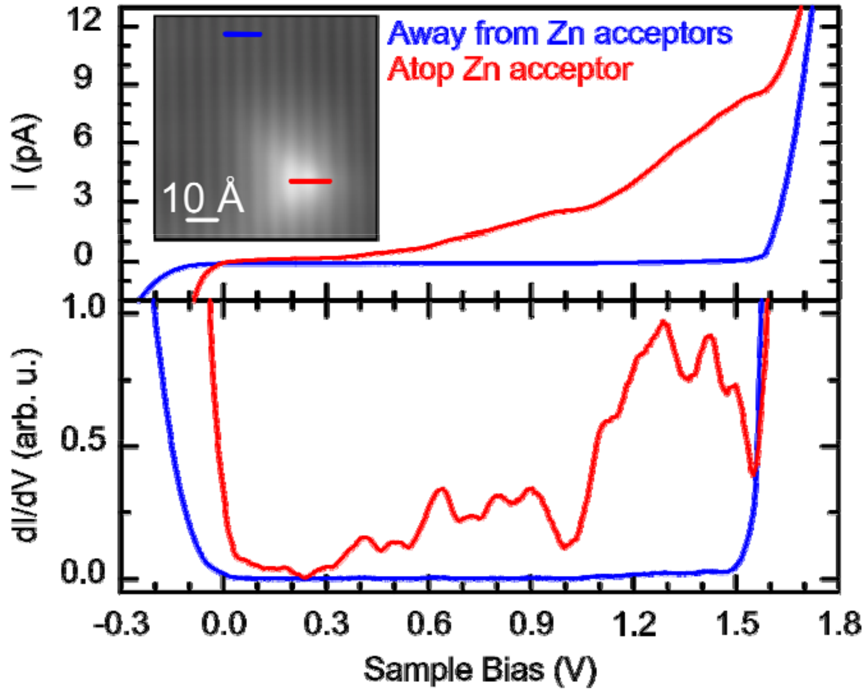
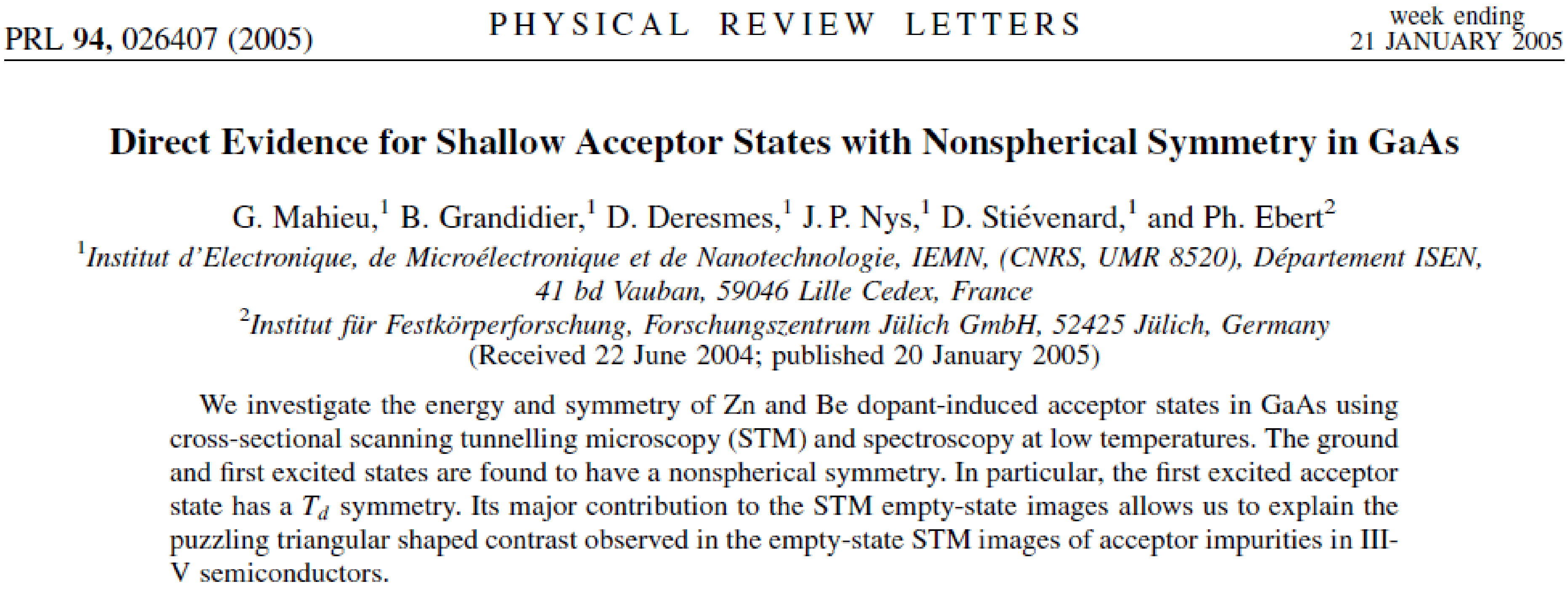




Literature Review: Zn in GaAs



PRL **94,** 026407 (2005) PHYSICAL REVIEW LETTERS week ending 21 JANUARY 2005

Direct Evidence for Shallow Acceptor States with Nonspherical Symmetry in GaAs

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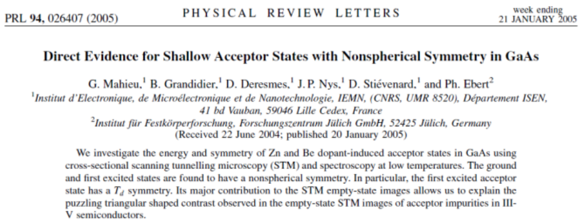

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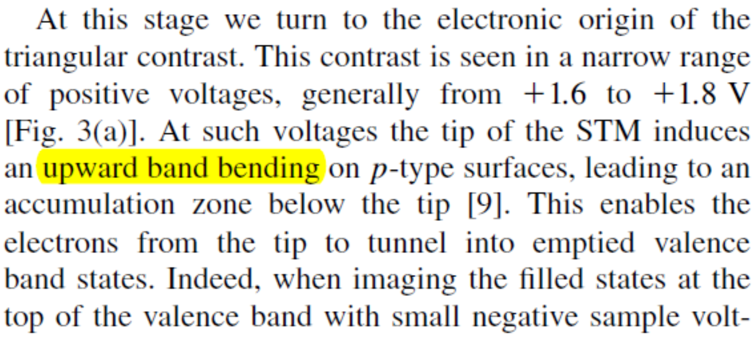
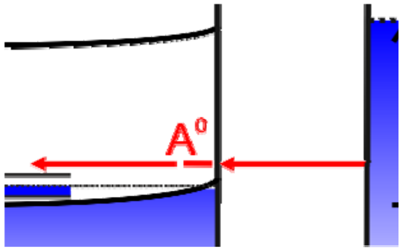


At this stage we turn to the electronic origin of the triangular contrast. This contrast is seen in a narrow range of positive voltages, generally from +1.6 to +1.8 V [Fig. 3(a)]. At such voltages the tip of the STM induces an upward band bending on p-type surfaces, leading to an accumulation zone below the tip [9]. This enables the electrons from the tip to tunnel into emptied valence band states. Indeed, when imaging the filled states at the top of the valence band with small negative sample volt-



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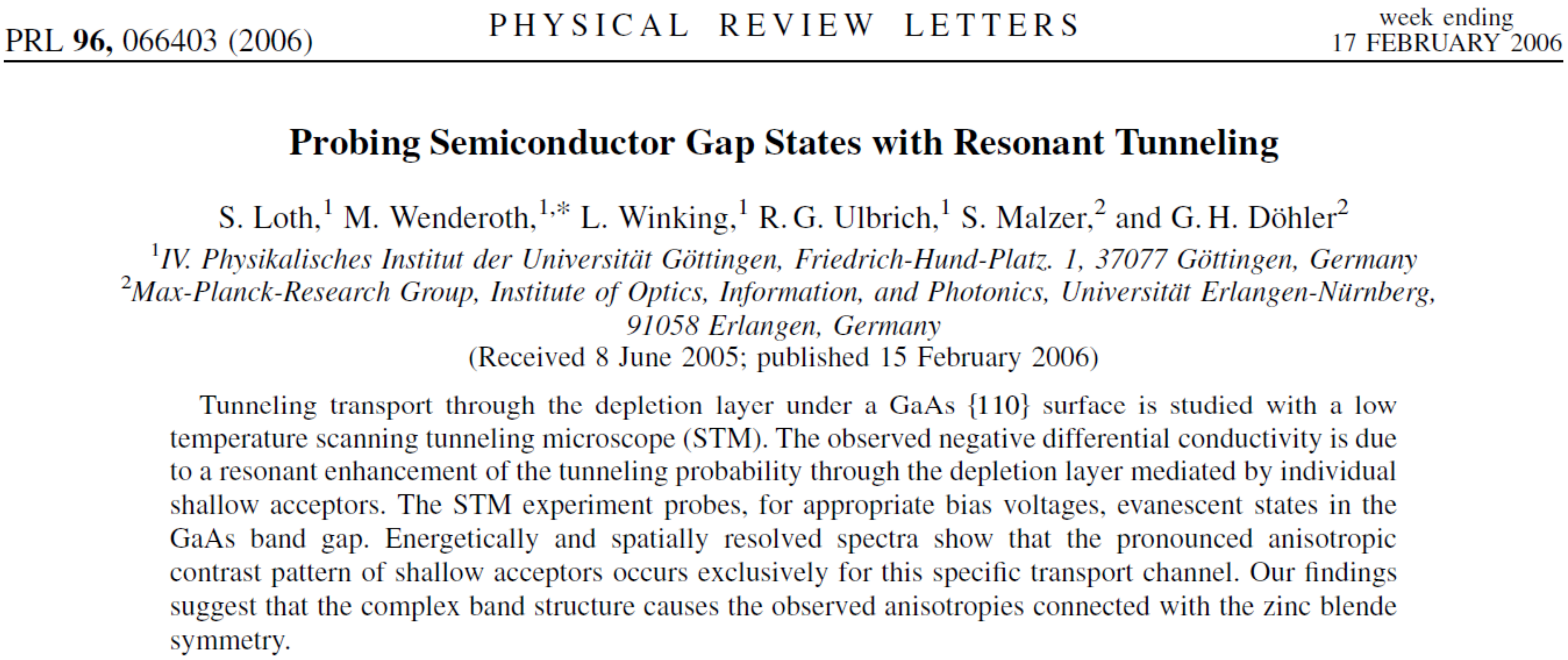

PRL **96,** 066403 (2006) PHYSICAL REVIEW LETTERS week ending 17 FEBRUARY 2006

Probing Semiconductor Gap States with Resonant Tunneling

S. Loth,[1] M. Wenderoth,[1,*] L. Winking,[1] R. G. Ulbrich,[1] S. Malzer,[2] and G. H. Döhler[2]
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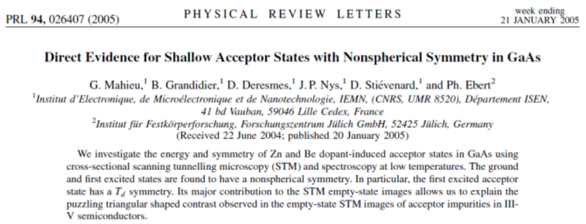
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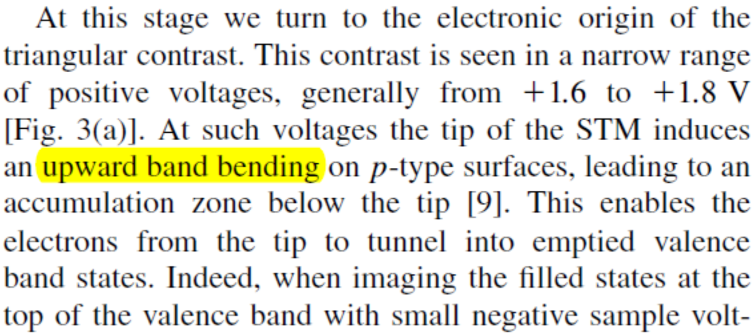
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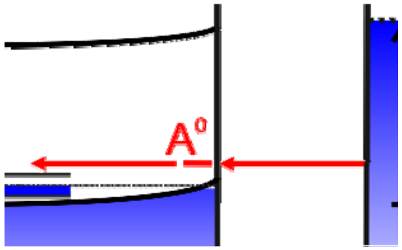

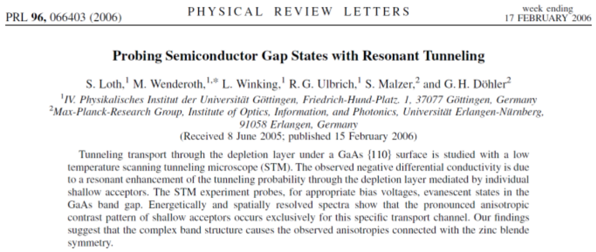
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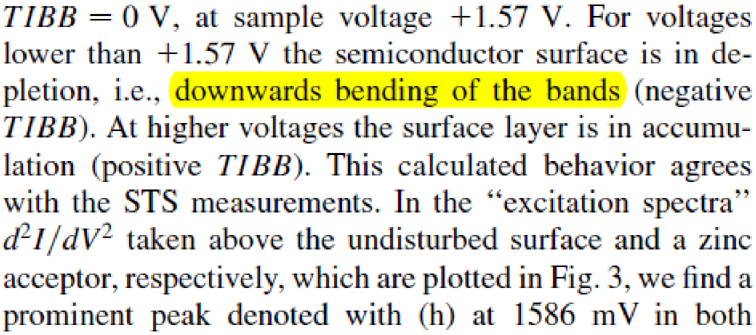
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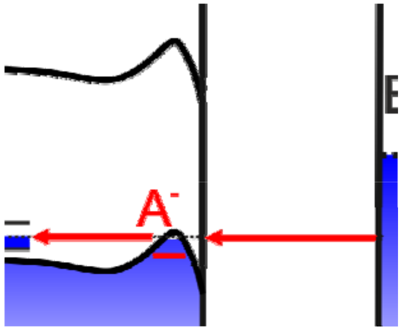
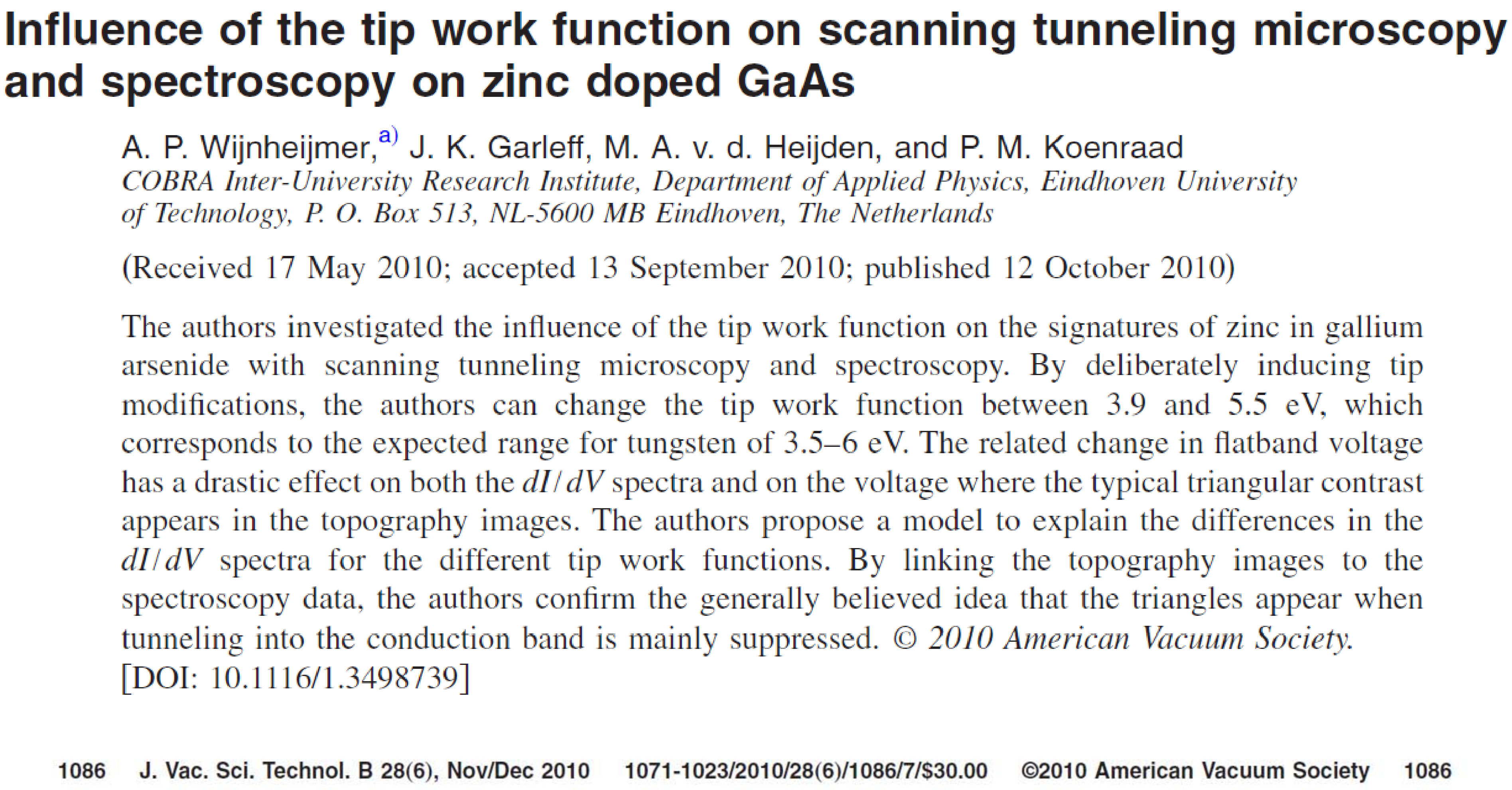


Literature Review: Zn in GaAs



Influence of the tip work function on scanning tunneling microscopy and spectroscopy on zinc doped GaAs

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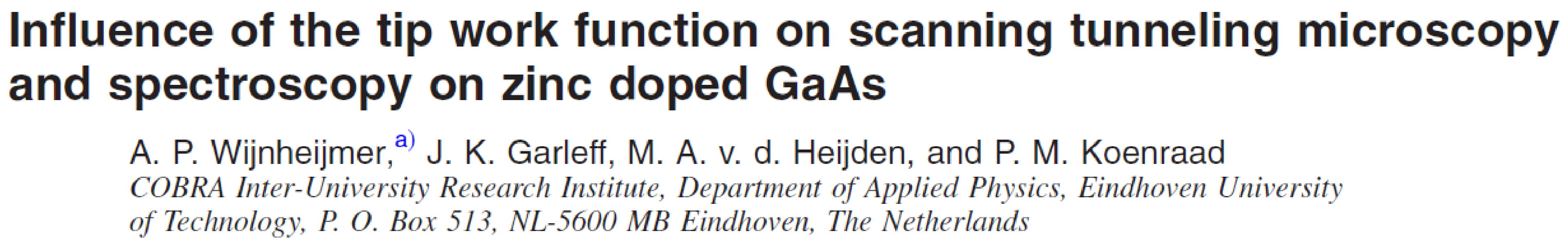
COBRA Inter-University Research Institute, Department of Applied Physics, Eindhoven University of Technology, P. O. Box 513, NL-5600 MB Eindhoven, The Netherlands

(Received 17 May 2010; accepted 13 September 2010; published 12 October 2010)

The authors investigated the influence of the tip work function on the signatures of zinc in gallium arsenide with scanning tunneling microscopy and spectroscopy. By deliberately inducing tip modifications, the authors can change the tip work function between 3.9 and 5.5 eV, which corresponds to the expected range for tungsten of 3.5–6 eV. The related change in flatband voltage has a drastic effect on both the dI/dV spectra and on the voltage where the typical triangular contrast appears in the topography images. The authors propose a model to explain the differences in the dI/dV spectra for the different tip work functions. By linking the topography images to the spectroscopy data, the authors confirm the generally believed idea that the triangles appear when tunneling into the conduction band is mainly suppressed. © *2010 American Vacuum Society.*
[DOI: 10.1116/1.3498739]

1086 J. Vac. Sci. Technol. B 28(6), Nov/Dec 2010 1071-1023/2010/28(6)/1086/7/$30.00 ©2010 American Vacuum Society 1086

Literature Review: Zn in GaAs



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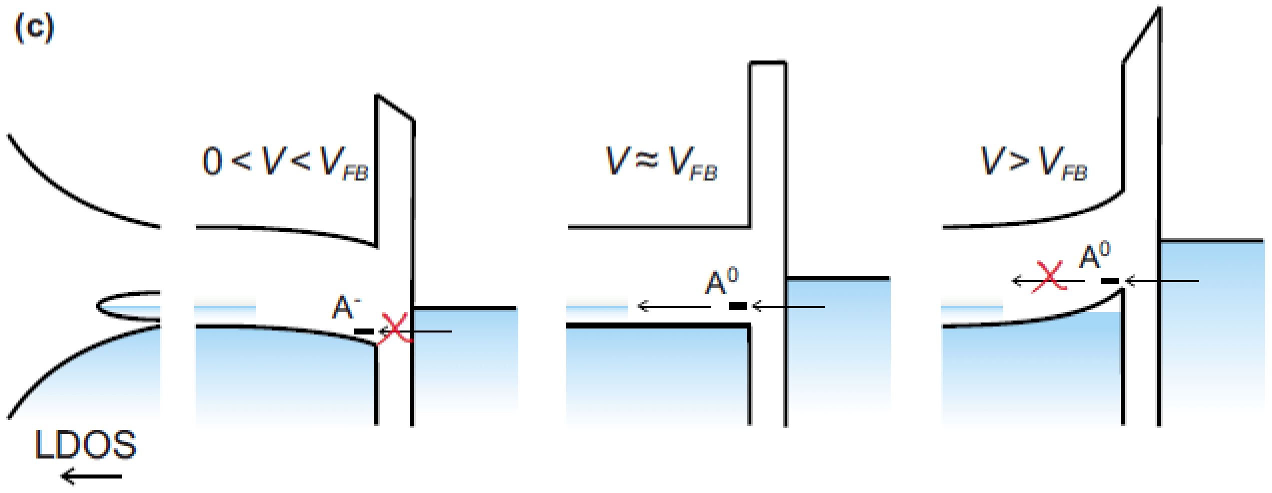

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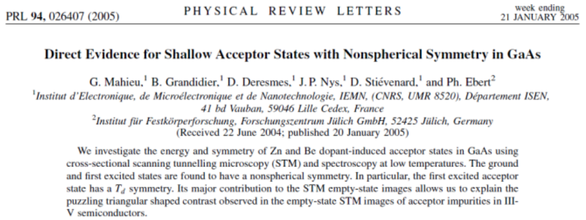
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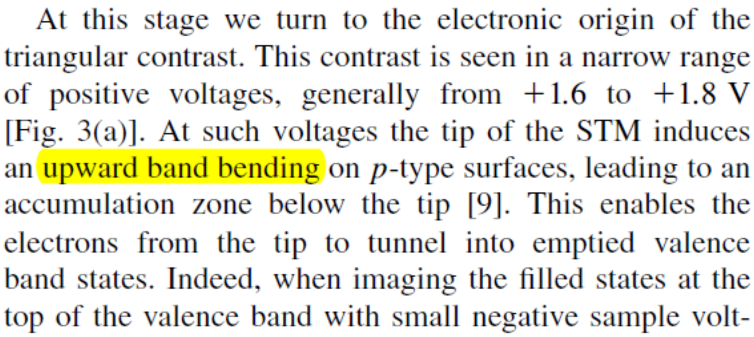
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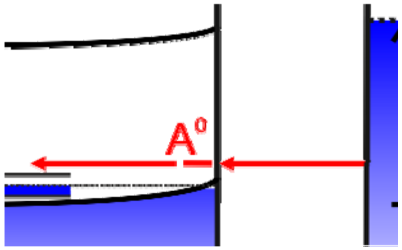

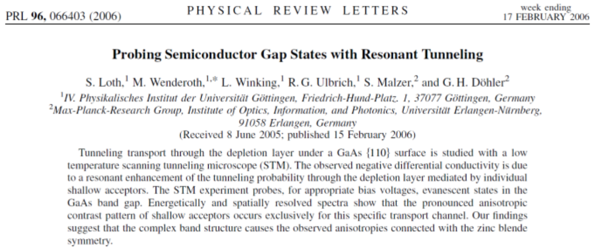
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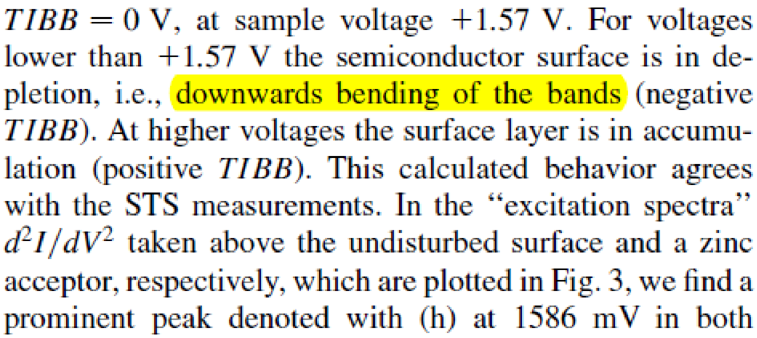
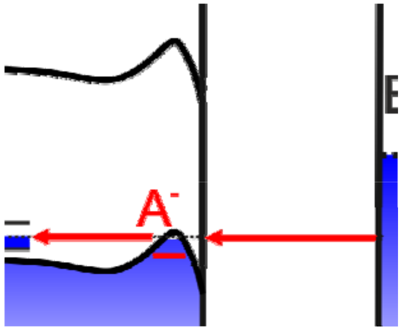
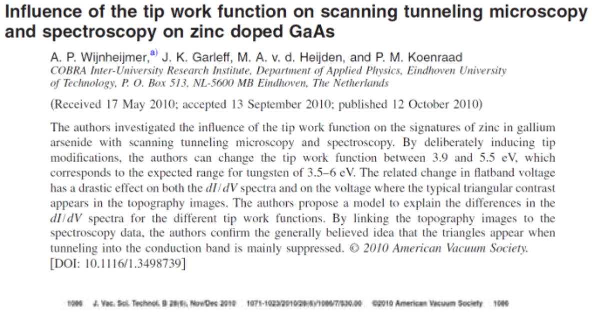

$TIBB = 0$ V, at sample voltage $+1.57$ V. For voltages lower than $+1.57$ V the semiconductor surface is in depletion, i.e., downwards bending of the bands (negative $TIBB$). At higher voltages the surface layer is in accumulation (positive $TIBB$). This calculated behavior agrees with the STS measurements. In the "excitation spectra" d^2I/dV^2 taken above the undisturbed surface and a zinc acceptor, respectively, which are plotted in Fig. 3, we find a prominent peak denoted with (h) at 1586 mV in both




Influence of the tip work function on scanning tunneling microscopy and spectroscopy on zinc doped GaAs

A. P. Wijnheijmer,[a)] J. K. Garleff, M. A. v. d. Heijden, and P. M. Koenraad
COBRA Inter-University Research Institute, Department of Applied Physics, Eindhoven University of Technology, P. O. Box 513, NL-5600 MB Eindhoven, The Netherlands

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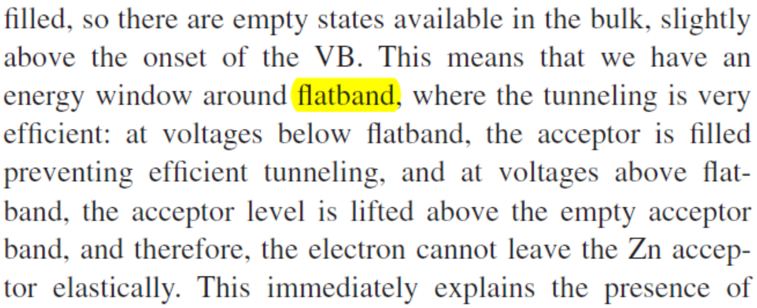
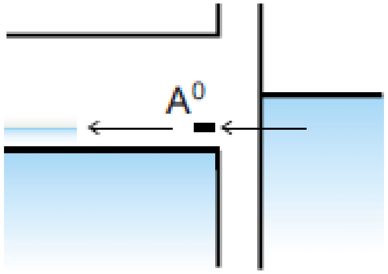
The authors investigated the influence of the tip work function on the signatures of zinc in gallium arsenide with scanning tunneling microscopy and spectroscopy. By deliberately inducing tip modifications, the authors can change the tip work function between 3.9 and 5.5 eV, which corresponds to the expected range for tungsten of 3.5–6 eV. The related change in flatband voltage has a drastic effect on both the dI/dV spectra and on the voltage where the typical triangular contrast appears in the topography images. The authors propose a model to explain the differences in the dI/dV spectra for the different tip work functions. By linking the topography images to the spectroscopy data, the authors confirm the generally believed idea that the triangles appear when tunneling into the conduction band is mainly suppressed. © *2010 American Vacuum Society.* [DOI: 10.1116/1.3498739]

1086 J. Vac. Sci. Technol. B 28(6), Nov/Dec 2010 1071-1023/2010/28(6)/1086/7/$30.00 ©2010 American Vacuum Society 1086


filled, so there are empty states available in the bulk, slightly above the onset of the VB. This means that we have an energy window around flatband, where the tunneling is very efficient: at voltages below flatband, the acceptor is filled preventing efficient tunneling, and at voltages above flatband, the acceptor level is lifted above the empty acceptor band, and therefore, the electron cannot leave the Zn acceptor elastically. This immediately explains the presence of



Literature Review: Zn in GaAs - Summary

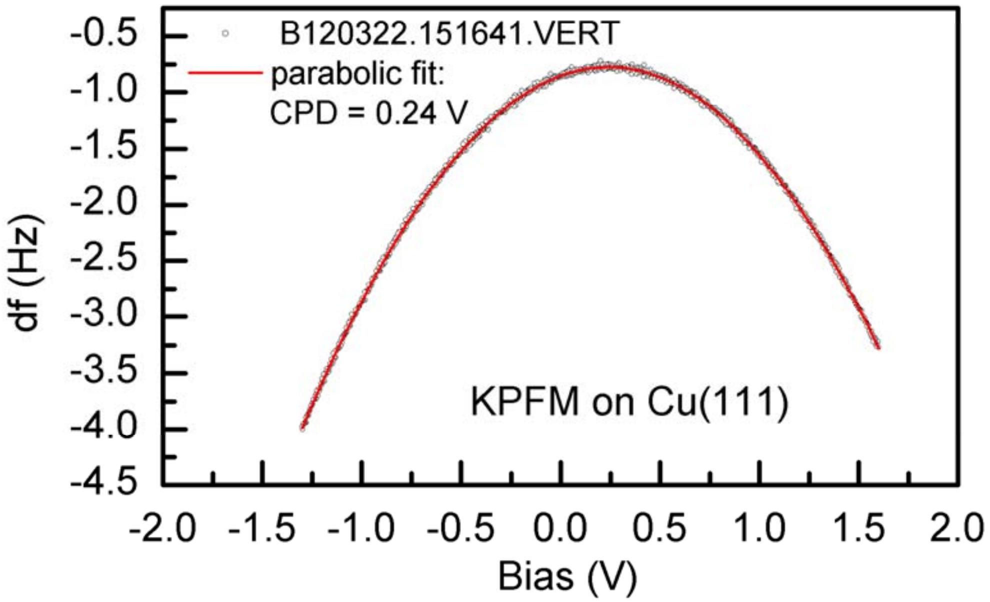
In-gap acceptor-related enhanced current and conductance is observed.

All papers either guess the tip's work function or extract it from I(z), which is known to give only a rough estimate for Φ_{tip} (*J. Phys. Chem. C.* ***113****, 11301 (2009)*).

The explanations given are based on single particle pictures of transport.

However: In using combined X-STM/AFM, we have an exact method to determine the tip's work function: **KPFM**

Kelvin Probe Force Microscopy (KPFM)



Setpoint: U_{bias} = 50 mV, I = 2.5 pA,
Δz = -5 Å, A_{oszi} = 1 Å

→ **the maximum in KPFM signal corresponds to CPD**

- Energy of capacitor: $E = \frac{1}{2} C \cdot V^2$

  V: voltage drop between tip and sample $V = CPD/e + V_{Bias}$

- frequency shift $df = \frac{\partial F}{\partial z} = -\frac{\partial^2}{\partial z^2} E$
- df(V) is parabolic in V:

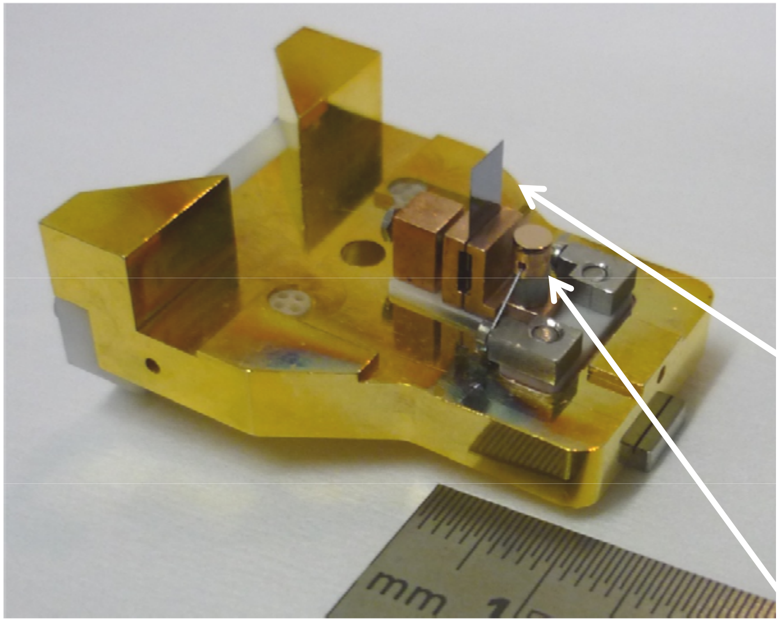
$$df = \frac{\partial F}{\partial z} = -\frac{1}{2}\frac{\partial^2 C}{\partial z^2} \cdot (CPD/e + V_{Bias})^2$$

- the maxima of the parabola is located at:

$$V_{Bias} = -CPD/e$$

Appl. Phys. Lett. **58**, 2921 (1991)

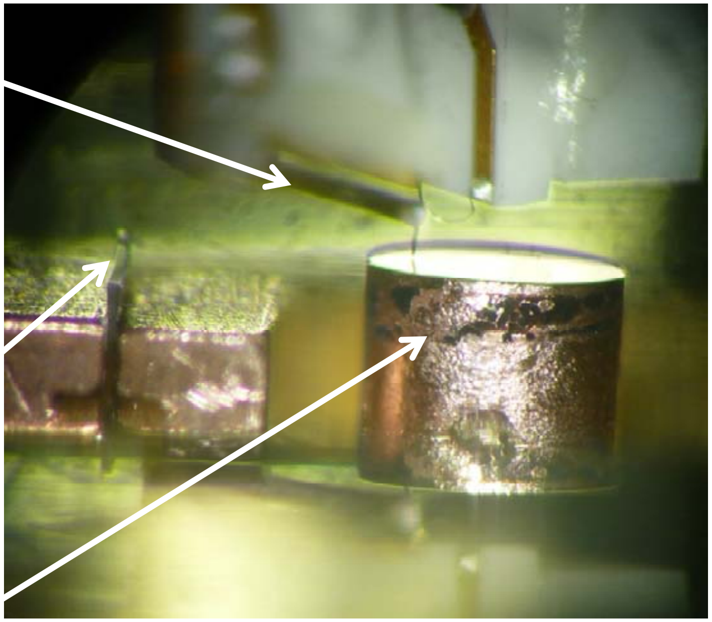
Dual sample holder



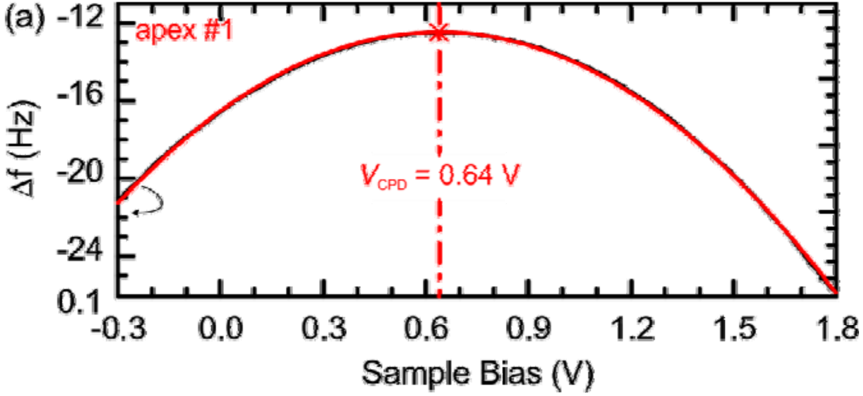
tuning fork

wafer

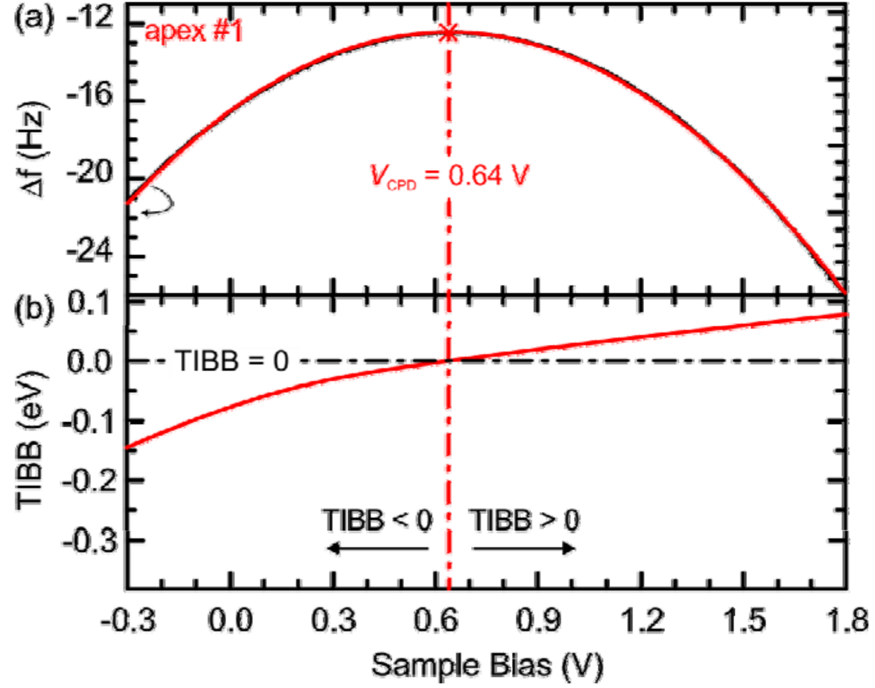
Cu-crystal



Cu single-crystal and wafer are accessible within one experiment.

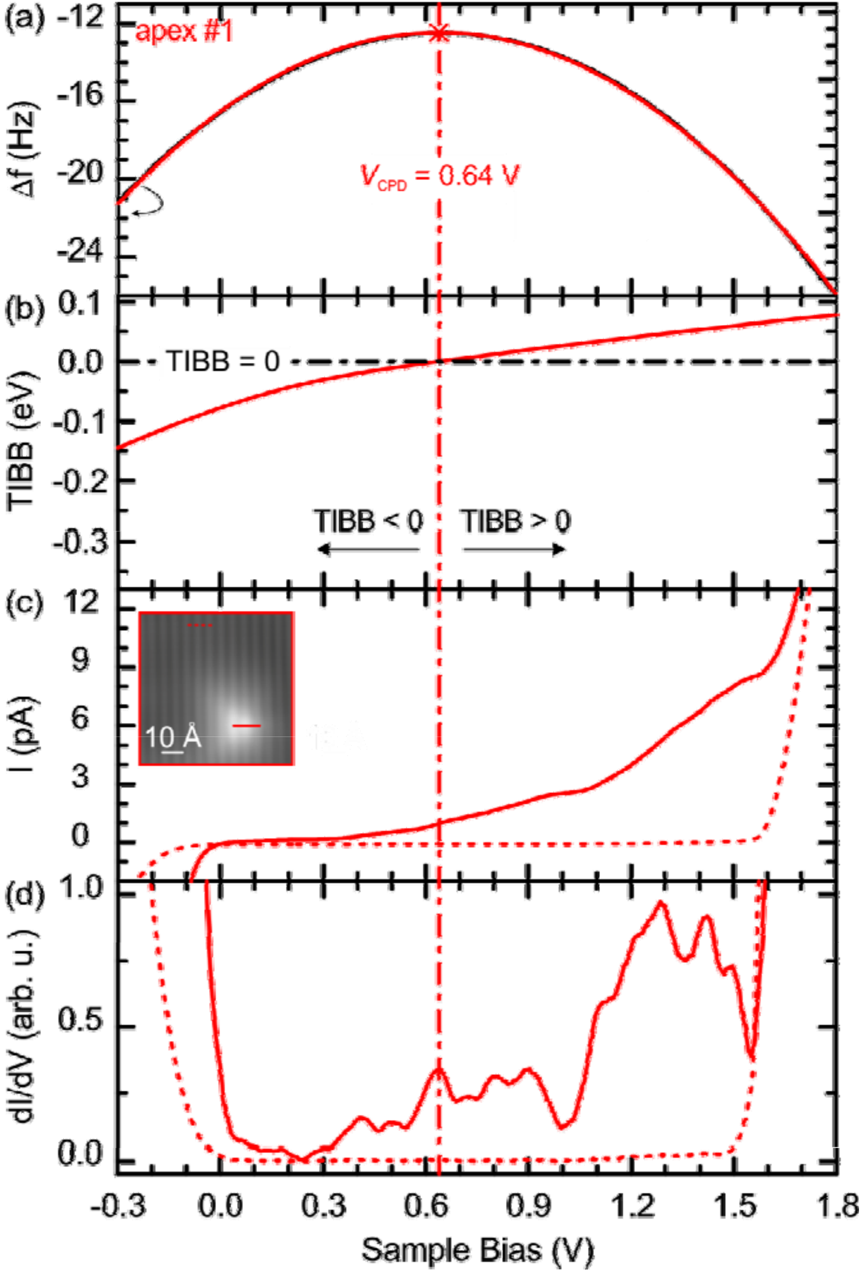


From KPFS, we determine V_{CPD} for a particular tip apex, V_{CPD} = 0.64 V



From KPFS, we determine V_{CPD} for a particular tip apex, V_{CPD} = 0.64 V

Calculate TIBB(V), using a Poisson equation solver with V_{CPD} as input

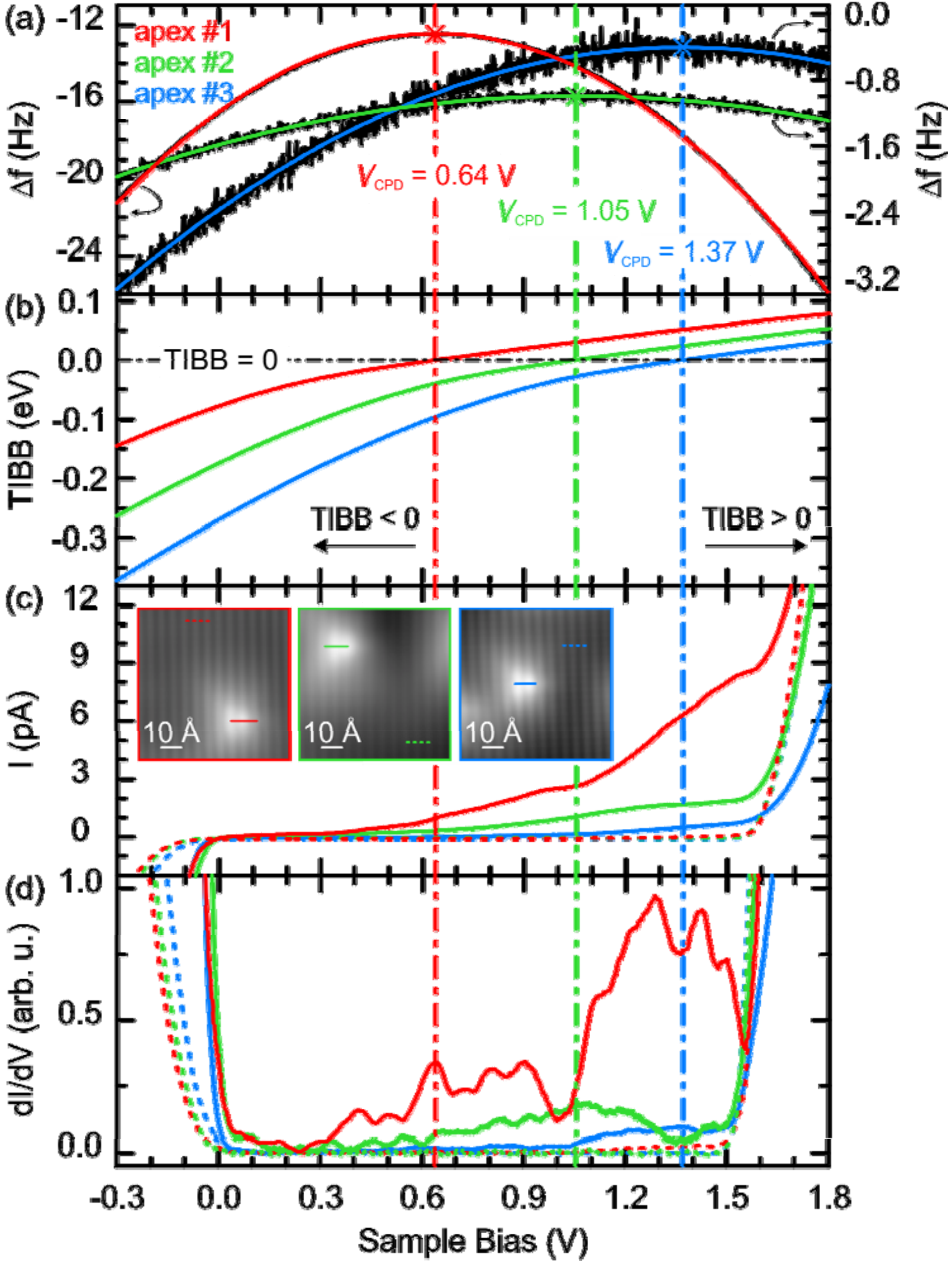


From KPFS, we determine V_{CPD} for a particular tip apex, V_{CPD} = 0.64 V

Calculate TIBB(V), using a Poisson equation solver with V_{CPD} as input parameter

STS related to the flat-band voltage

Enhanced Acceptor related current is present in negative, zero and positive TIBB regimes



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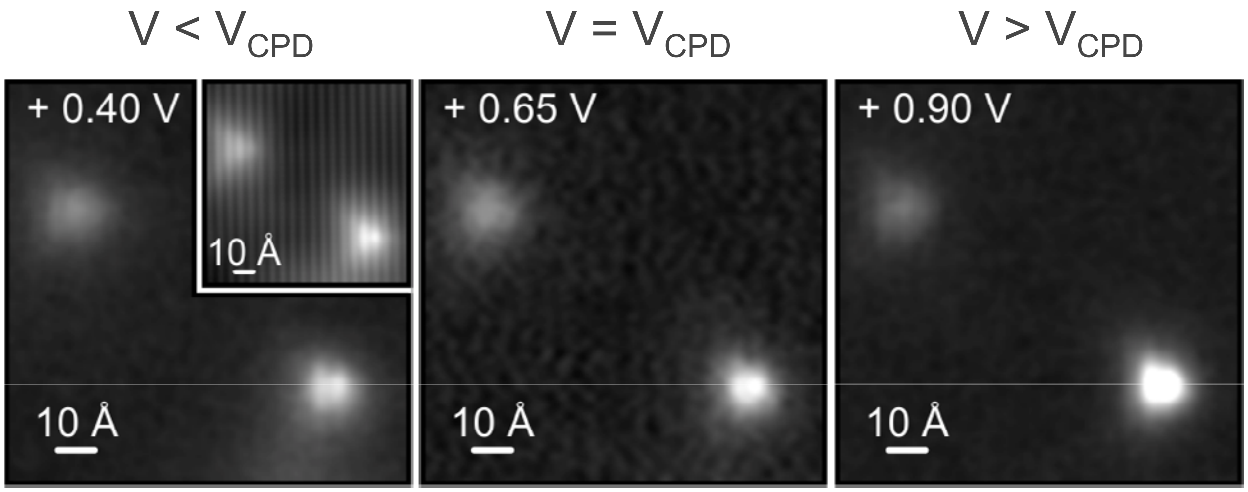
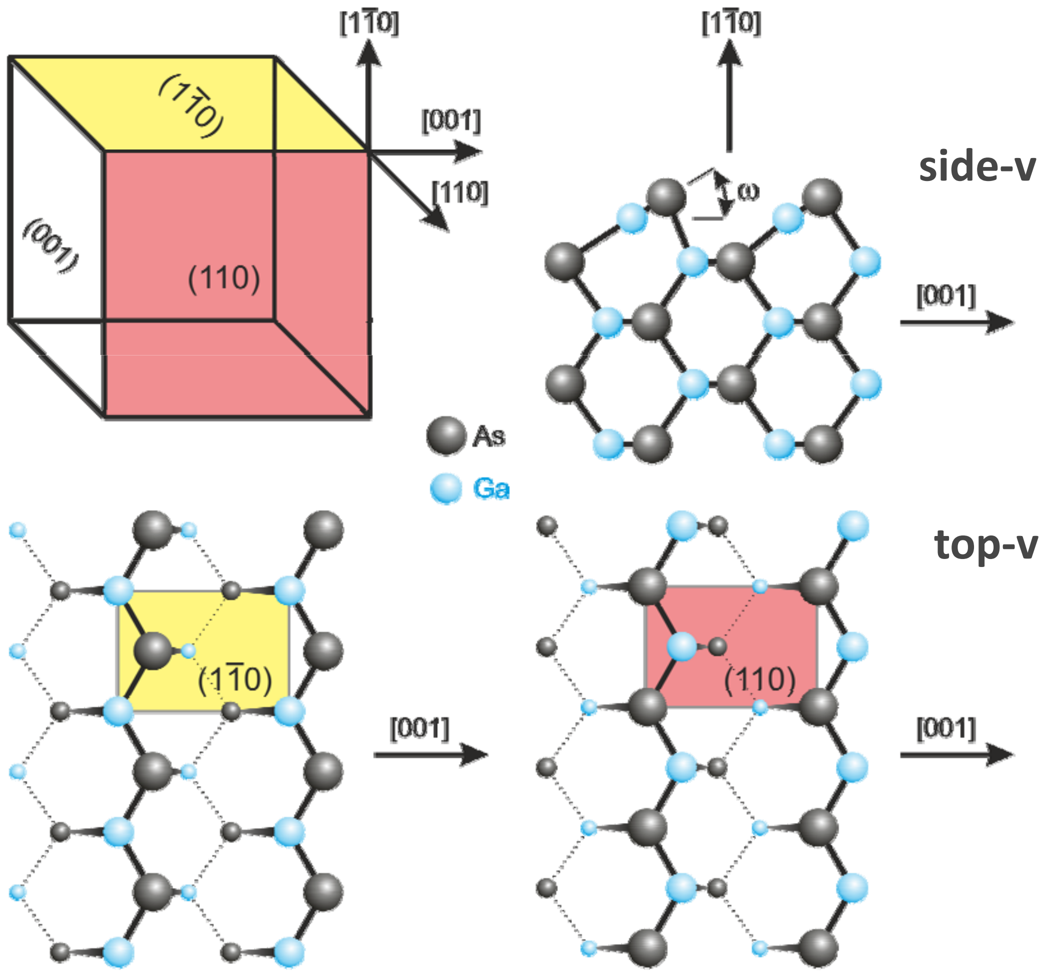


Constant-height dI/dV maps reveal a similar triangular feature of enhanced conductance in negative, zero and positive TIBB regimes

One conduction mechanism in active in all three band bending regimes

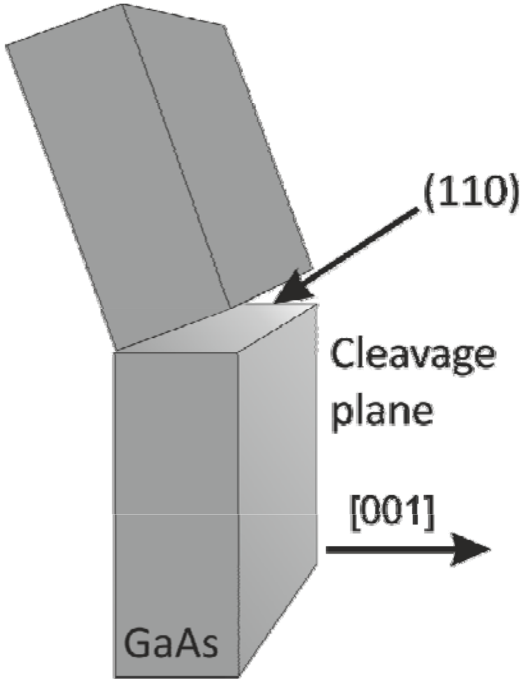
The {110} surfaces of GaAs

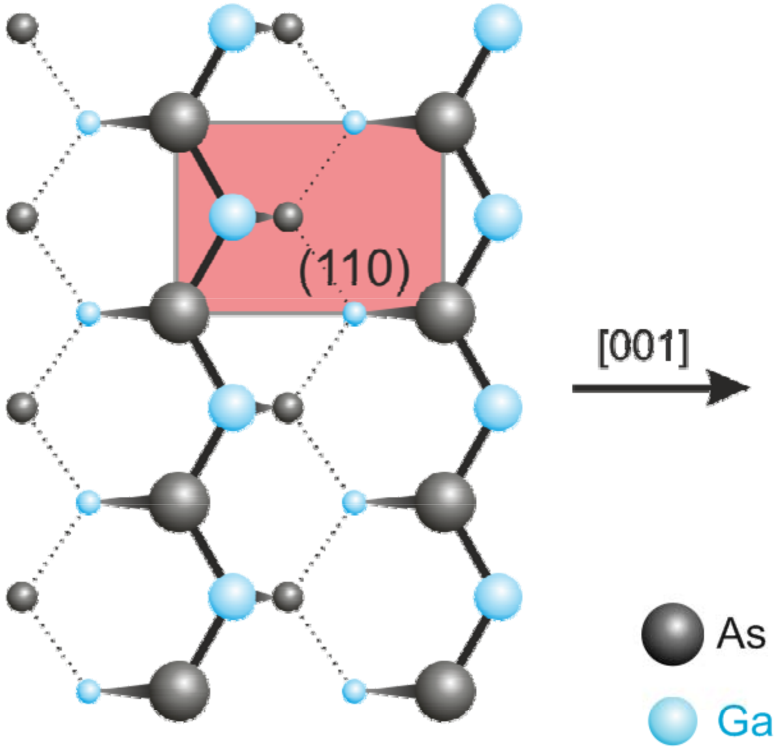


side-view

top-view

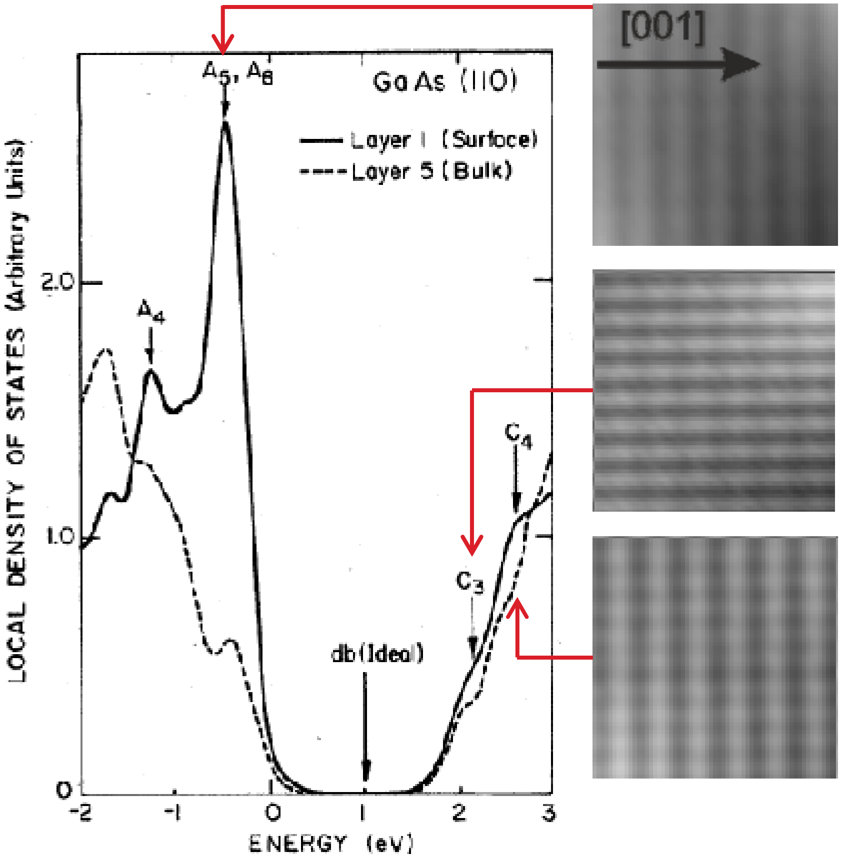
Crystallographic properties of GaAs





GaAs: III-V semiconductor, zinc-blende lattice structure.
(110) surface: prepared by cleaving of wafer, consists of alternating rows of As and Ga atoms

Electronic properties of GaAs(110)



A5
U_{bias} = - 0.5 V

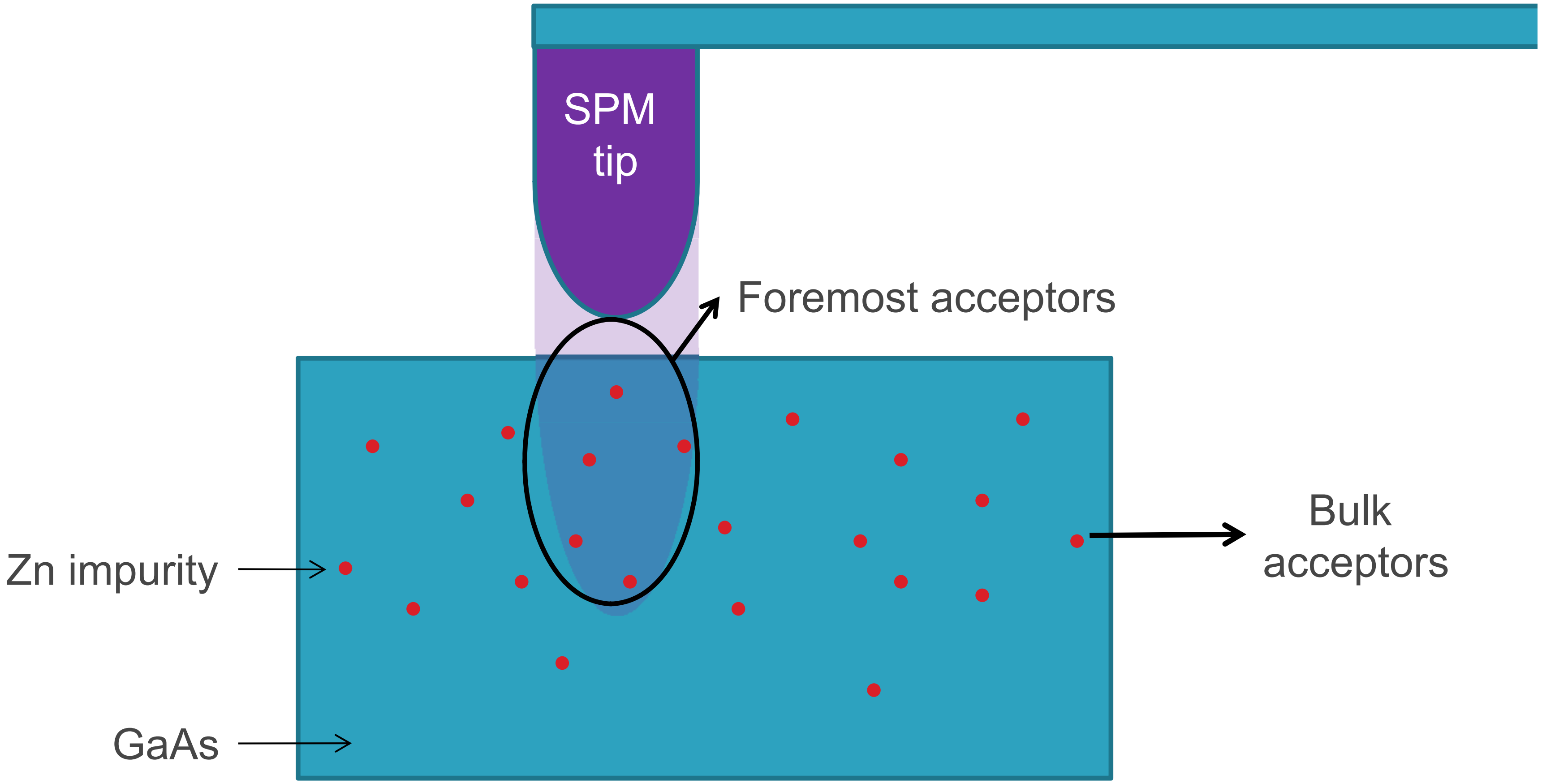
C3
U_{bias} = + 1.6 V

C4
U_{bias} = + 2.2 V

calculated DOS: Phys. Rev. B **20**, 4150 (1979)

- 4 surface resonances outside the band gap
- Fermi-level not pinned:
  -> tunneling is only possible
  for certain bias voltages
  -> bulk DOS is not masked
- Resonances have the same spatial periodicity as surface unit cell
- A5 and C4: rows perpendicular to [001]
  C3: rows parallel to [001]

Bulk vs. Foremost acceptors



The Hamiltonian for the junction

$$H = H_{\mathrm{acc}} + H_{\mathrm{sub}} + H_{\mathrm{tip}} + H_{\mathrm{tun}}$$

Foremost acceptors (FA)

Interacting electrons
Anderson-Hubbard model

Substrate:
Bulk acceptors + semiconductor

Non-interacting electrons with energy dependent DOS

Metallic tip

Non-interacting electrons with flat DOS

Tunnelling between previous blocks

Single particle
Geometrical encoded

Anderson-Hubbard model

$$H_{\mathrm{acc}} = \sum_{i=1}^{N} \sum_{\sigma} \epsilon_i c_{i\sigma}^{\dagger} c_{i\sigma} + t \sum_{i=1}^{N-1} \sum_{\sigma} \left(c_{i\sigma}^{\dagger} c_{(i+1)\sigma} + c_{(i+1)\sigma}^{\dagger} c_{i\sigma} \right)$$

$$+ U \sum_{i=1}^{N} \left(c_{i\uparrow}^{\dagger} c_{i\uparrow} - \tfrac{1}{2} \right) \left(c_{i\downarrow}^{\dagger} c_{i\downarrow} - \tfrac{1}{2} \right)$$

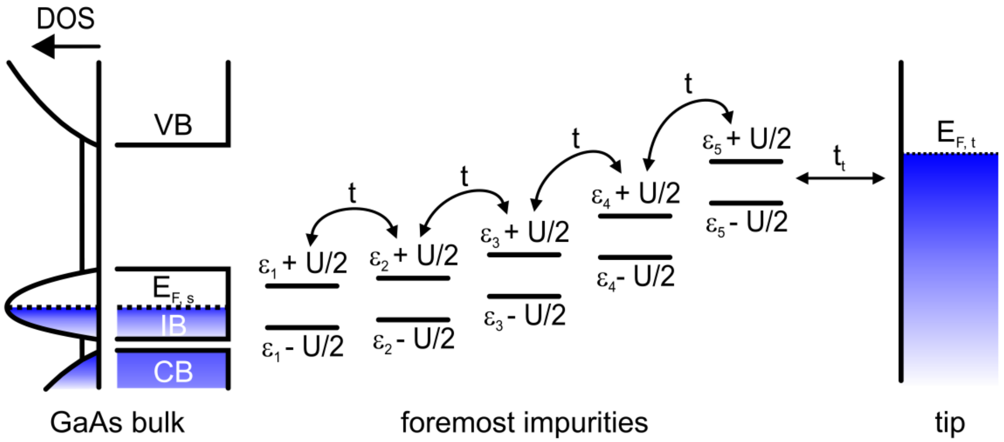
$$t = -5\mathrm{meV}$$

$$U = 10 - 20\mathrm{meV}$$

⇧

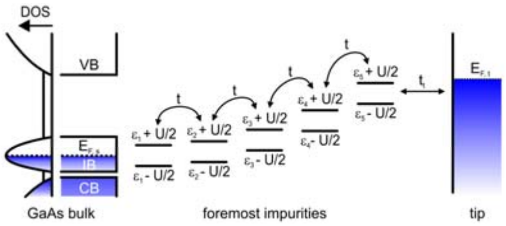
$$a_{\mathrm{B}} = 20\text{Å}$$

$$\varepsilon_r = 13$$



$$\epsilon_i = \mu_0 + \left(\frac{i-1}{N-1} \right)^2 TIBB(V)$$

Anderson-Hubbard model



We considered 5 acceptor states

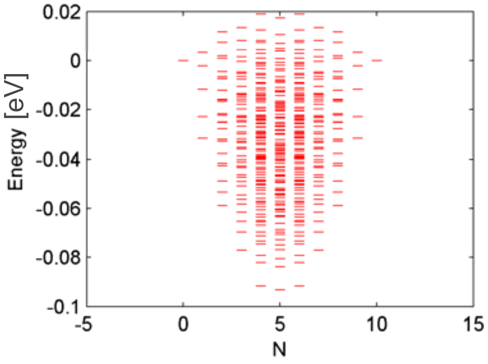
The number of states in the Fock space of the system is $4^5 = 1024$

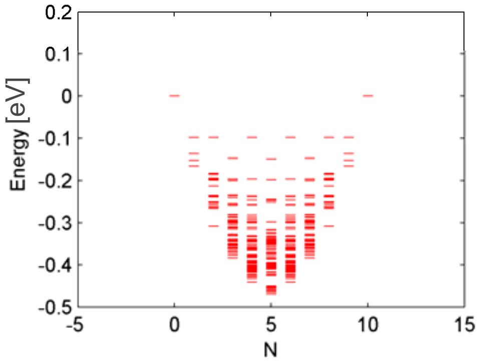
The system Hamiltonian is particle-hole symmetric

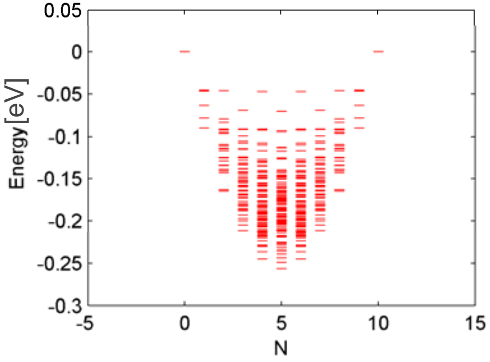
- In equilibrium: Number of electrons = number of impurities
- Constant terms in the interaction: positive ions at the acceptor sites
- Charge neutrality is accounted for

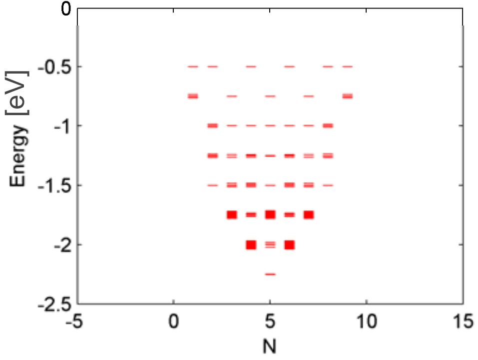
Spectrum of the Anderson-Hubbard Hamiltonians

t = -1 meV


U = |t|


U = 10|t|


U = 5|t|

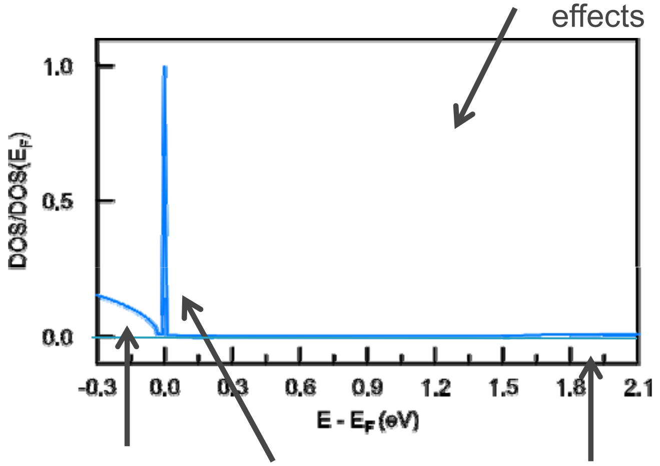

U = 50|t|

Particle-hole symmetry

Interplay of the hopping and charging dynamics for U ≤ 10|t|

Leads modeling

Substrate



Inelastic effects

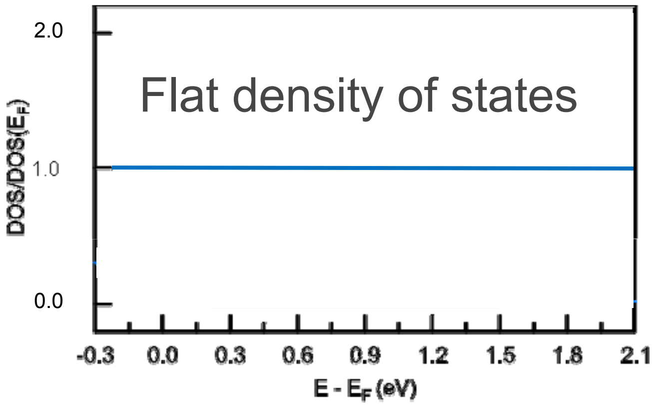
Valence band

Acceptors band

Conductance band

Free electron gas with:
Chemical potential μ_0
Temperture T

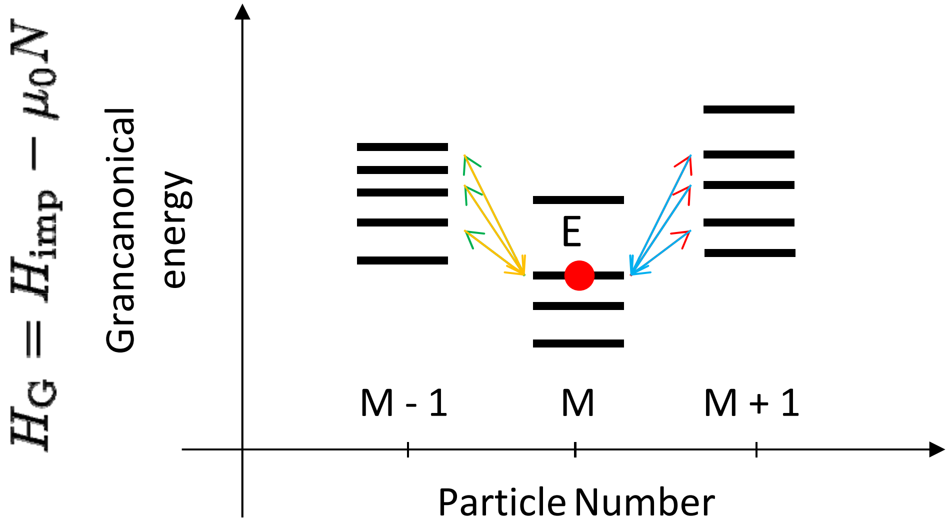
Tip



Flat density of states

Free electron gas with:
Chemical potential $\mu_0 - eV_b$
Temperture T

Transport: master equation approach



$$\dot{P}_{ME} = -\sum_{\chi E'} \left(R^{\chi}_{ME \to (M+1)E'} + R^{\chi}_{ME \to (M-1)E'}\right) P_{ME}$$

$$+ \sum_{\chi E'} R^{\chi}_{(M+1)E' \to ME} P_{(M+1)E'} + \sum_{\chi E'} R^{\chi}_{(M-1)E' \to ME} P_{(M-1)E'}$$

Tunnelling rates

Bias dependent

The **many-body rates** read

$$R^{\chi}_{ME\to(M+1)E'} = \sum_{\sigma}\sum_{i=1}^{N}\Gamma_i^{\chi}(E'-E)|\langle(M+1)E'|d^{\dagger}_{i\sigma}|ME\rangle|^2 f^{+}(E'-E-\mu_{\chi})$$

$$R^{\chi}_{ME\to(M-1)E'} = \sum_{\sigma}\sum_{i=1}^{N}\Gamma_i^{\chi}(E-E')|\langle(M-1)E'|d_{i\sigma}|ME\rangle|^2 f^{-}(E-E'-\mu_{\chi})$$

And contain the energy dependent **single particle rates**

Bias dependent

$$\Gamma_i^S(\Delta E) = \frac{2\pi}{\hbar}|t_S|^2 D_S(\Delta E)$$ ← Delocalization of the substrate tunnelling

$$\Gamma_i^T(\Delta E) = \frac{2\pi}{\hbar}|t_T|^2 D_T \delta_{iN}$$ ← Localization of the tip tunnelling to the last impurity

$$|t_S|^2/|t_T|^2 \approx 10^4$$ ← Extreme asymmetry in the coupling

$$\Gamma^T \approx 0.1\mu\text{eV}$$ → Estimated from the current

Average current

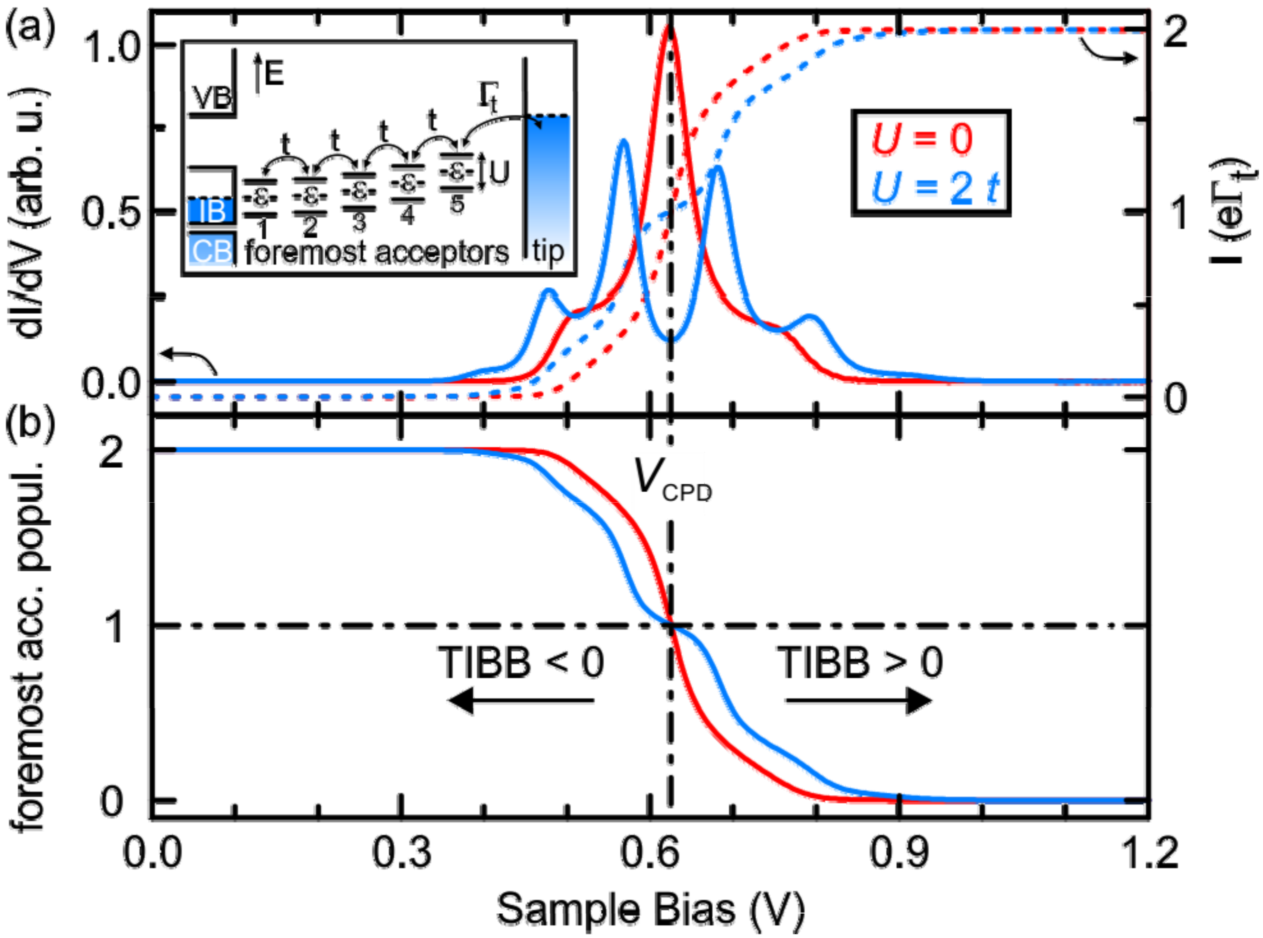
The average stationary current through the junction is calculated as:

$$
\begin{aligned}
I_T = \sum_{MEE'} M \big[&-(R^T_{ME\to(M+1)E'} + R^T_{ME\to(M-1)E'})P^{\mathrm{stat}}_{ME} \\
&+ R^T_{(M+1)E'\to ME}P^{\mathrm{stat}}_{(M+1)E'} + R^S_{(M-1)E'\to ME}P^{\mathrm{stat}}_{(M-1)E'})\big] \\
I_S = \sum_{MEE'} M \big[&-(R^S_{ME\to(M+1)E'} + R^S_{ME\to(M-1)E'})P^{\mathrm{stat}}_{ME} \\
&+ R^S_{(M+1)E'\to ME}P^{\mathrm{stat}}_{(M+1)E'} + R^S_{(M-1)E'\to ME}P^{\mathrm{stat}}_{(M-1)E'})\big]
\end{aligned}
$$

where one obtains due to charge conservation:

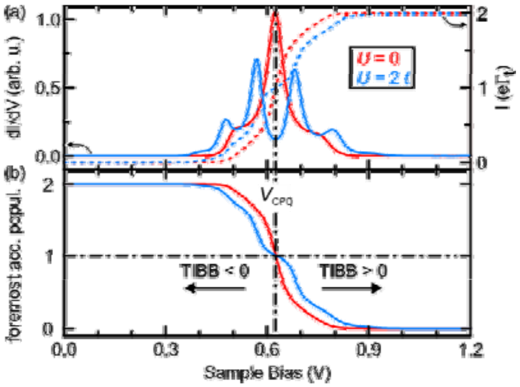
$$I_T = -I_S$$

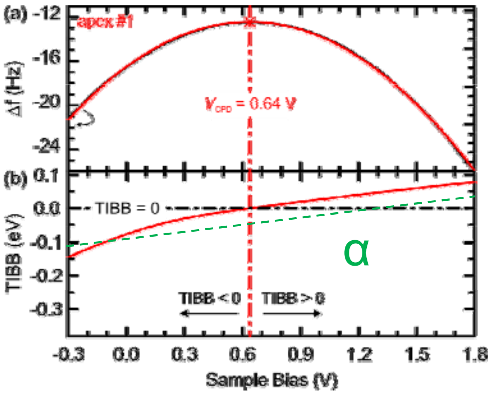
Current and differential conductance



Basic observations

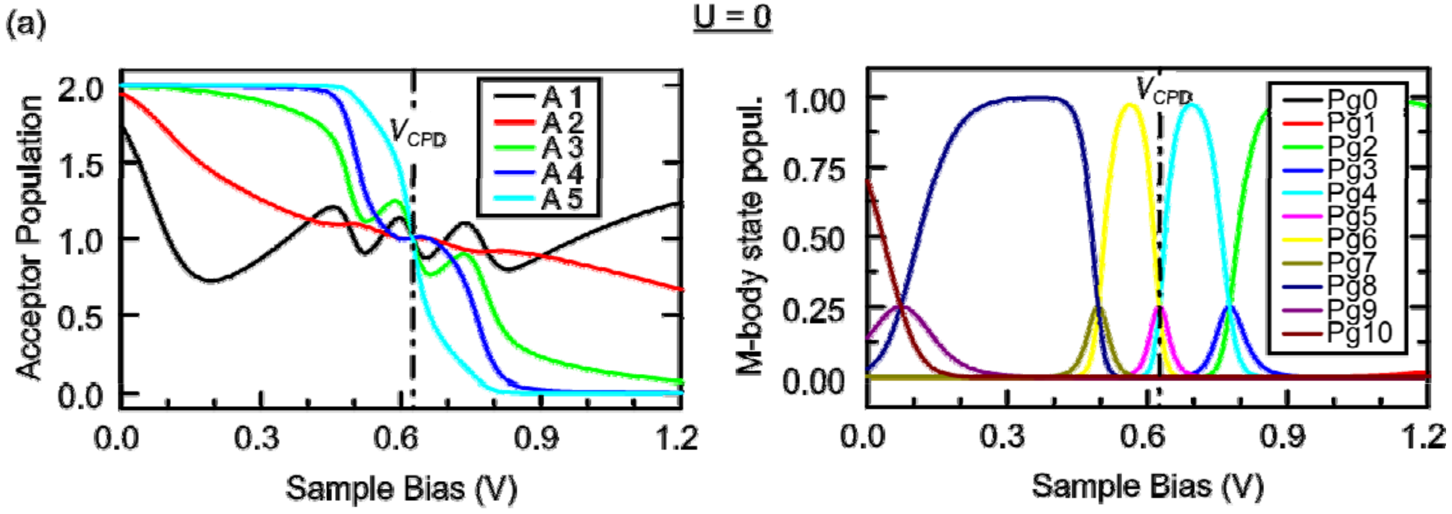
- Current flows through the system at $V_b > 0$ only if $N_5<2$
- At $U = 0$ the width of the current step is given by $4|t|/\alpha$
- At $U > 0$ a plateau develops around zero band bending, which increases with the strength of the interaction
- The finite current region becomes wider in presence of the interaction
- Reacher conduction structure appears in presence of the interaction



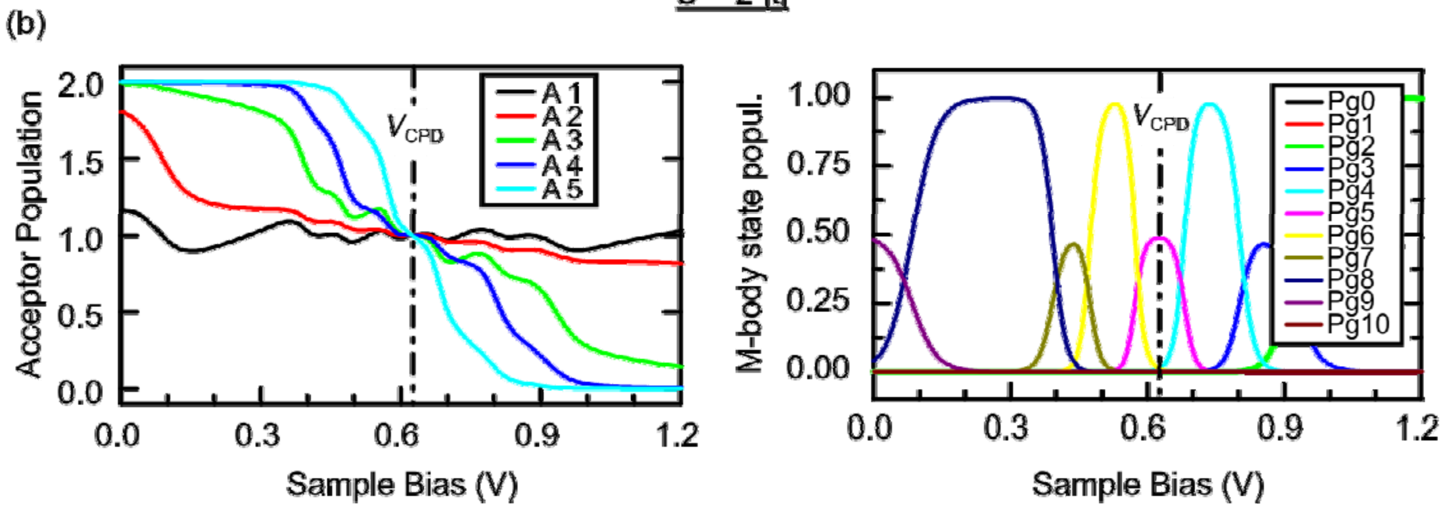


Impurities occupations and many-body states populations

U = 0



U = 2 |t|



Conclusions

- Due to the strong asymmetry between the tip and substrate coupling the system is always almost in equilibrium
- The current plateau around the zero band bending reflect the resistance of the system to charging , thus the size U/α
- A rich variety of peak structures in the differential conductance indicates the interplay between the coupling between the impurities and the charging energy
- An even richer variety expected for a more realistic 3D network of foremost impurities: each impurity has a different spectrum!

Thank you for your attention !