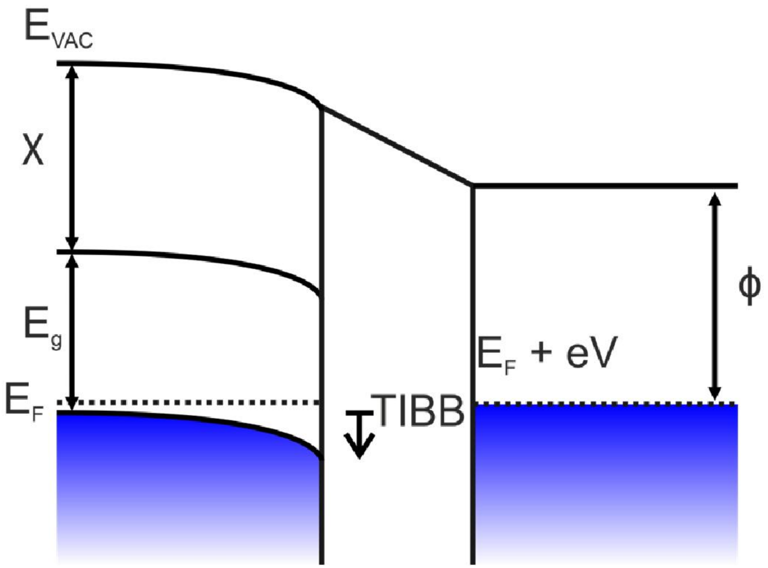
DPG meeting – Dresden 31.03.14

Fixing the energy scale in STM on semiconductor surfaces

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

GEORG-AUGUST-UNIVERSITÄT
GÖTTINGEN

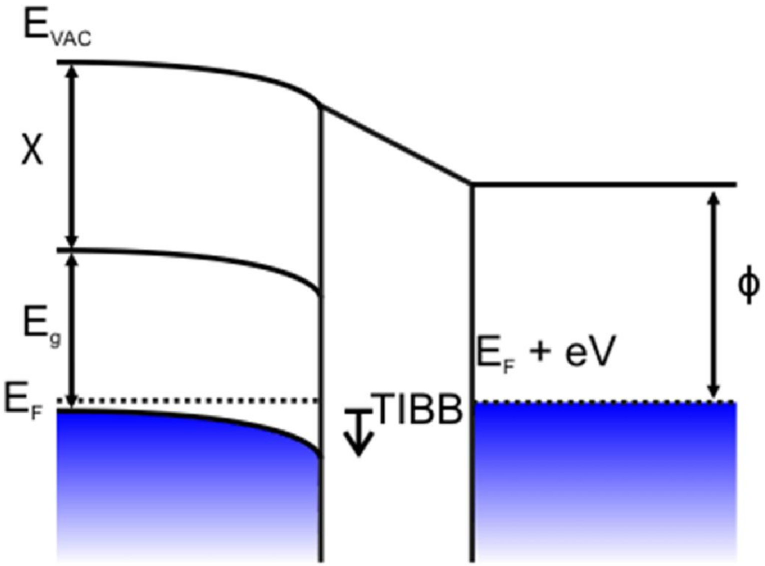
Tip induced band bending (TIBB)



- 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)

Tip induced band bending (TIBB)



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

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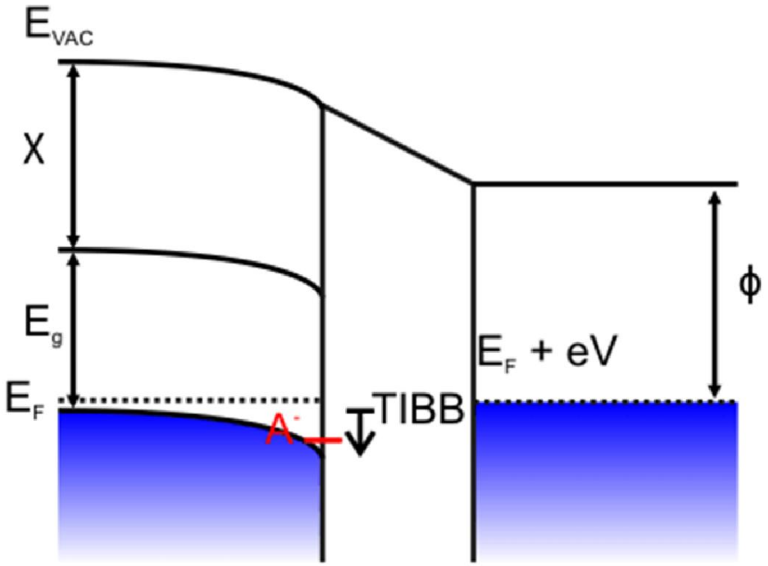

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- Electronic state can be shifted across the Fermi-level: Change of occupation $A^{-/0}$, change of contribution to tunneling

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

Tip induced band bending (TIBB)

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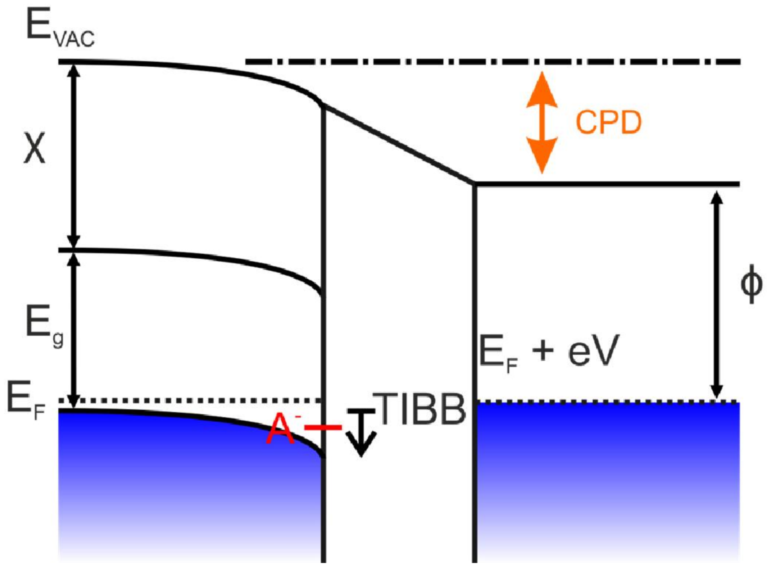
- TIBB(V) shifts the electronic position of all states below the tip

- 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 (CPD) between tip and sample



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

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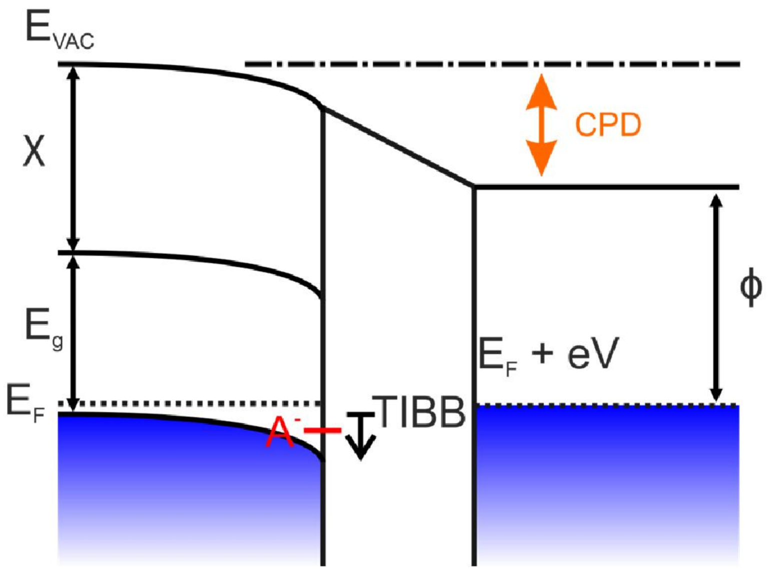
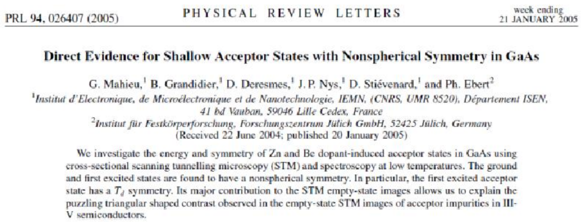
Tip induced band bending (TIBB)



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

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

Literature Review: Zn in GaAs



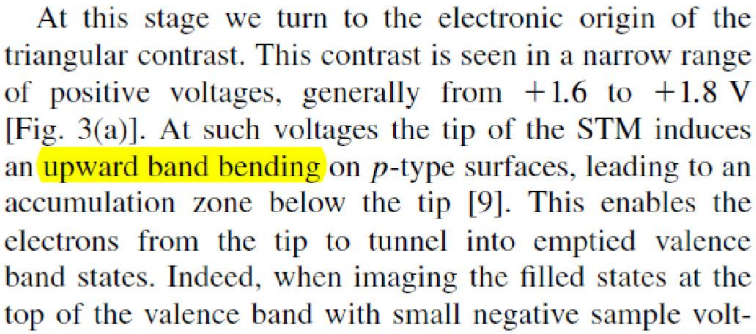
PRL 94, 026407 (2005) PHYSICAL REVIEW LETTERS week ending 21 JANUARY 2005

Direct Evidence for Shallow Acceptor States with Nonspherical Symmetry in GaAs

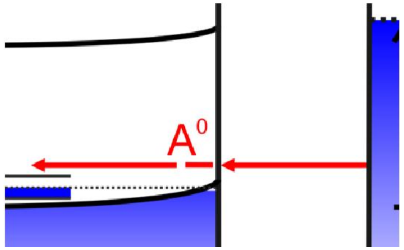
G. Mahieu,[1] B. Grandidier,[1] D. Deresmes,[1] J. P. Nys,[1] D. Stiévenard,[1] and Ph. Ebert[2]
[1]*Institut d'Electronique, de Microélectronique et de Nanotechnologie, IEMN, (CNRS, UMR 8520), Département ISEN, 41 bd Vauban, 59046 Lille Cedex, France*
[2]*Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany*
(Received 22 June 2004; published 20 January 2005)

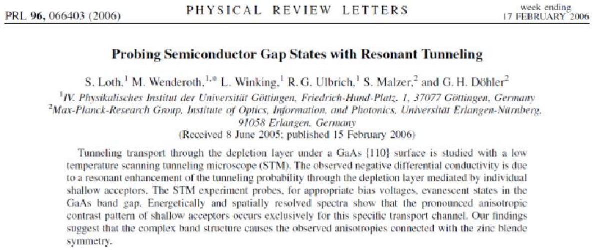
We investigate the energy and symmetry of Zn and Be dopant-induced acceptor states in GaAs using cross-sectional scanning tunnelling microscopy (STM) and spectroscopy at low temperatures. The ground and first excited states are found to have a nonspherical symmetry. In particular, the first excited acceptor state has a T_d symmetry. Its major contribution to the STM empty-state images allows us to explain the puzzling triangular shaped contrast observed in the empty-state STM images of acceptor impurities in III-V semiconductors.

PRL **94**, 026407 (2005)



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-





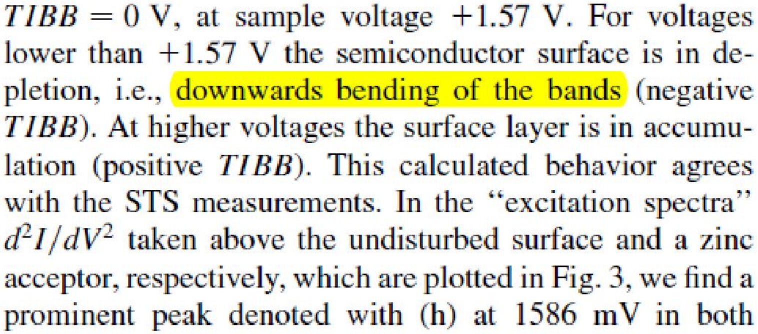
PRL 96, 066403 (2006) PHYSICAL REVIEW LETTERS week ending 17 FEBRUARY 2006

Probing Semiconductor Gap States with Resonant Tunneling

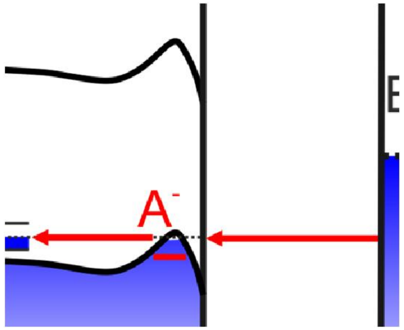
S. Loth,[1] M. Wenderoth,[1,*] L. Winking,[1] R. G. Ulbrich,[1] S. Malzer,[2] and G. H. Döhler[2]
[1]*IV. Physikalisches Institut der Universität Göttingen, Friedrich-Hund-Platz. 1, 37077 Göttingen, Germany*
[2]*Max-Planck-Research Group, Institute of Optics, Information, and Photonics, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany*
(Received 8 June 2005; published 15 February 2006)

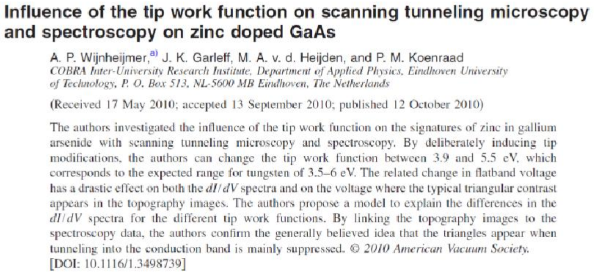
Tunneling transport through the depletion layer under a GaAs {110} surface is studied with a low temperature scanning tunneling microscope (STM). The observed negative differential conductivity is due to a resonant enhancement of the tunneling probability through the depletion layer mediated by individual shallow acceptors. The STM experiment probes, for appropriate bias voltages, evanescent states in the GaAs band gap. Energetically and spatially resolved spectra show that the pronounced anisotropic contrast pattern of shallow acceptors occurs exclusively for this specific transport channel. Our findings suggest that the complex band structure causes the observed anisotropies connected with the zinc blende symmetry.

PRL **96**, 066403 (2006)



$TIBB = 0$ 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





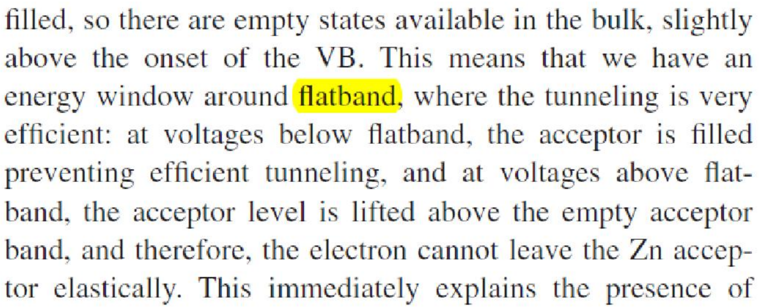
Influence of the tip work function on scanning tunneling microscopy and spectroscopy on zinc doped GaAs

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

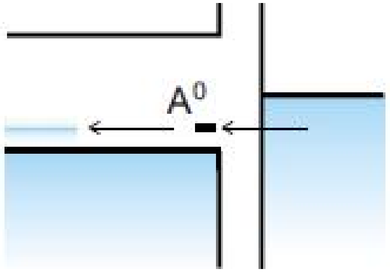
(Received 17 May 2010; accepted 13 September 2010; published 12 October 2010)

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]

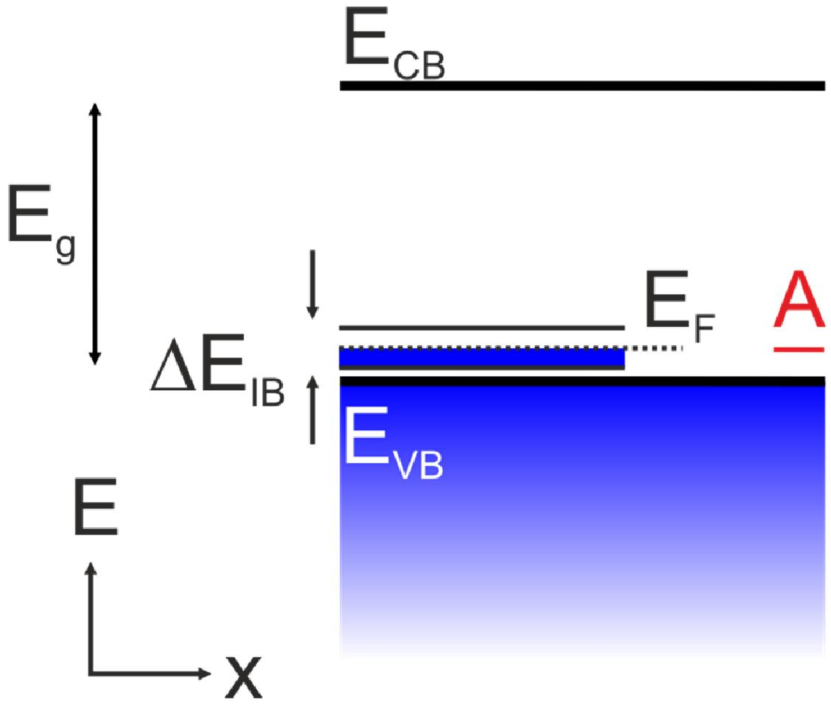
J. Vac. Sci. Technol. B **28** 1086 (2010)



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



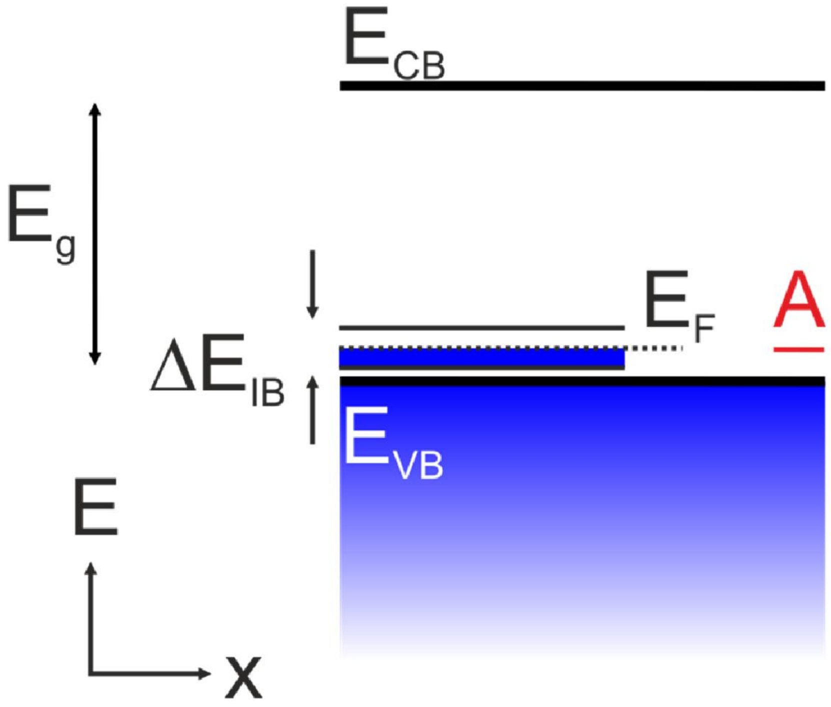
Electronic properties of Zn doped GaAs

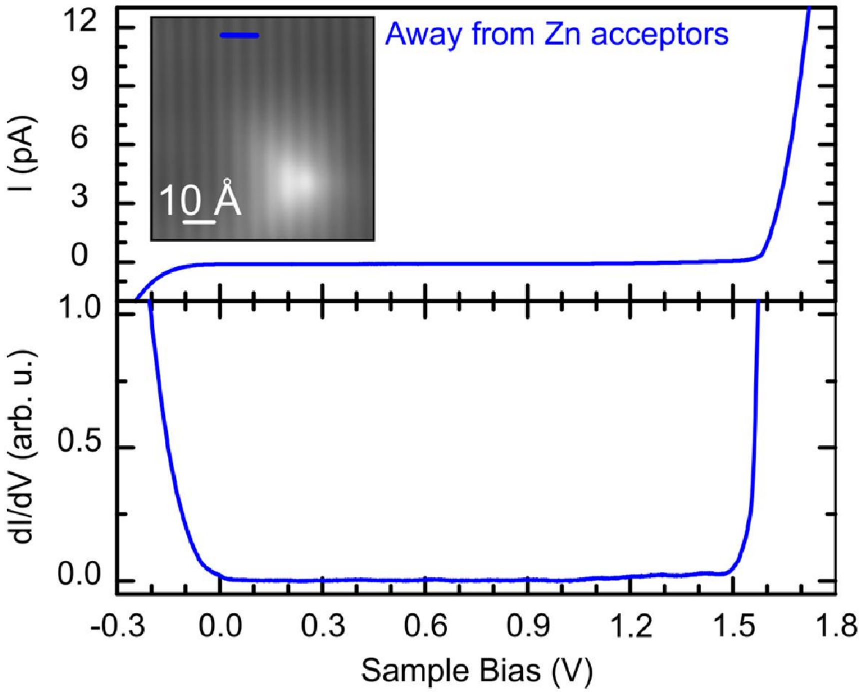


- Zn is an acceptor in GaAs -> p-type doping
- Zn ionization energy in GaAs: 31 meV
- For the dopant concentration $1 \cdot 10^{19}$ Zn/cm^3 used here impurity band of ΔE_{IB} = 24 meV width is established

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

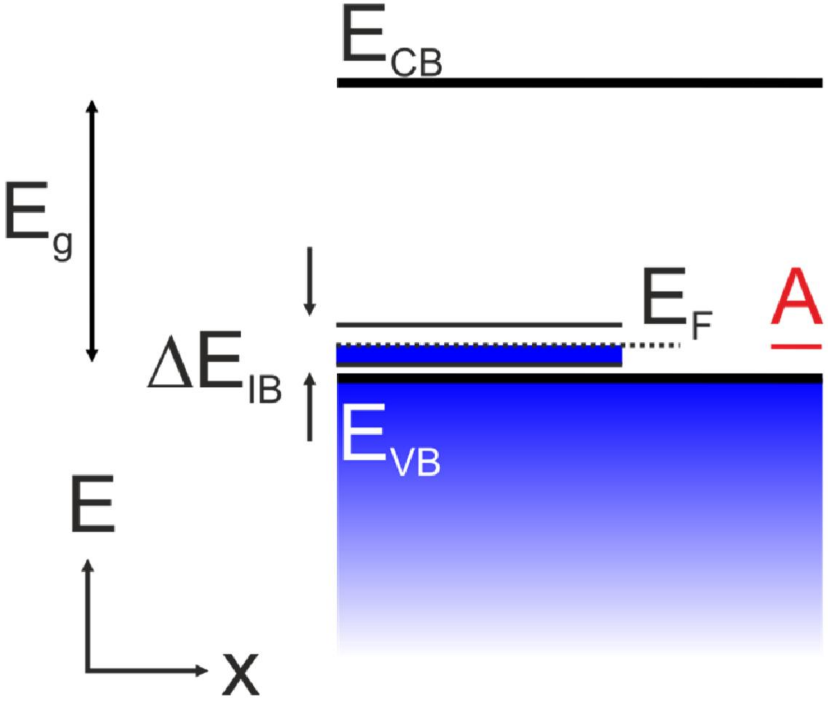
Electronic properties of Zn doped GaAs

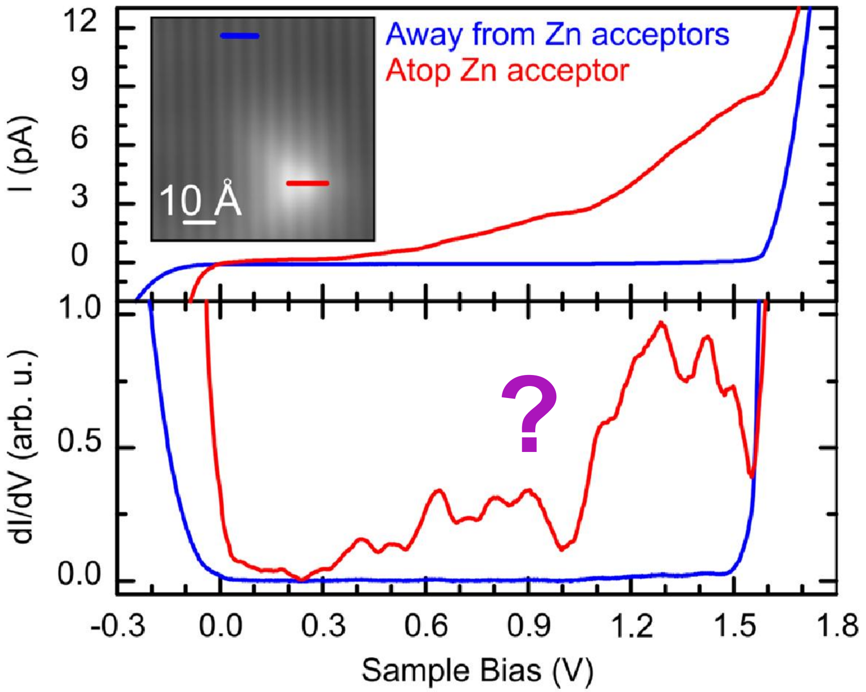




G. Münnich, A. Donarini, J. Repp, and M. Wenderoth, *Phys. Rev. Lett* **111**, 216802 (2013)

Electronic properties of Zn doped GaAs





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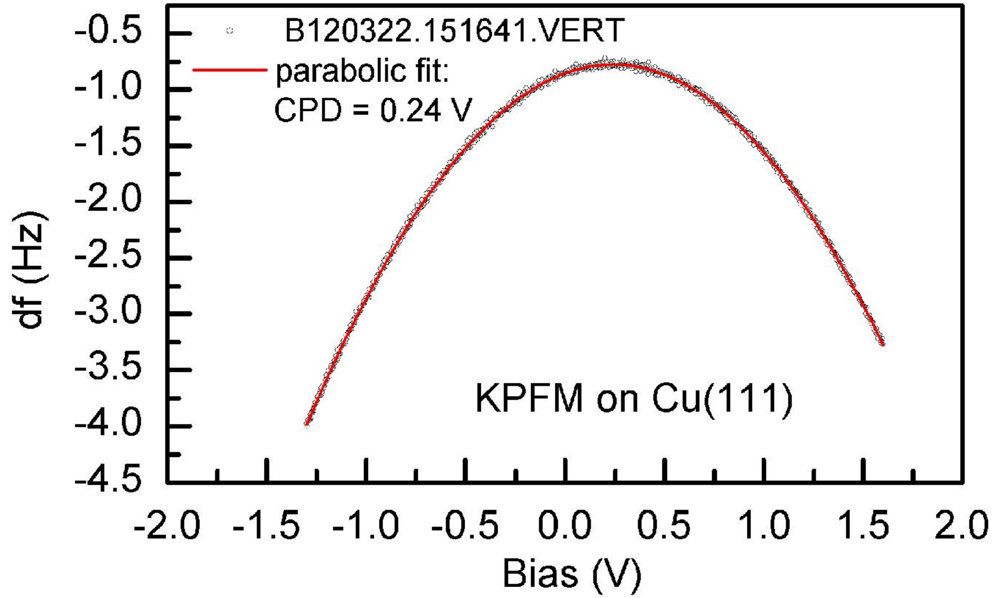
Simultaneous

Scanning **T**unnelling **M**icroscopy

and

Kelvin **P**robe **F**orce **M**icroscopy

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 $V = CPD/e + V_{Bias}$

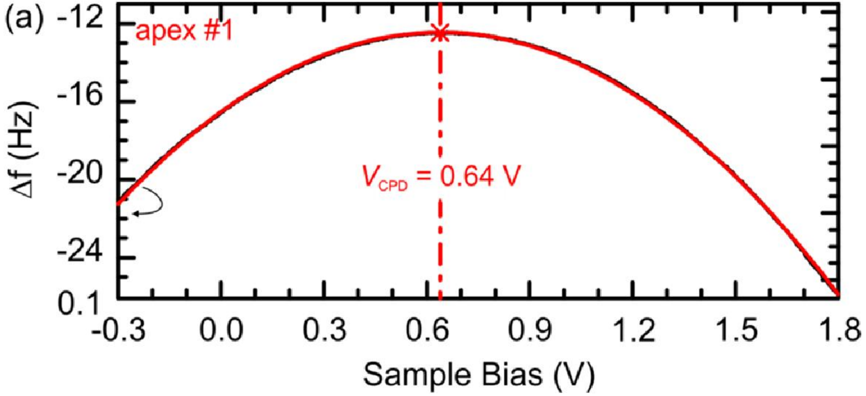
- frequency shift $df = \frac{\partial F}{\partial z} = -\frac{\partial^2}{\partial z^2} E$
- df(V) is parabolic in V:

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

- the maximum of the parabola is located at:

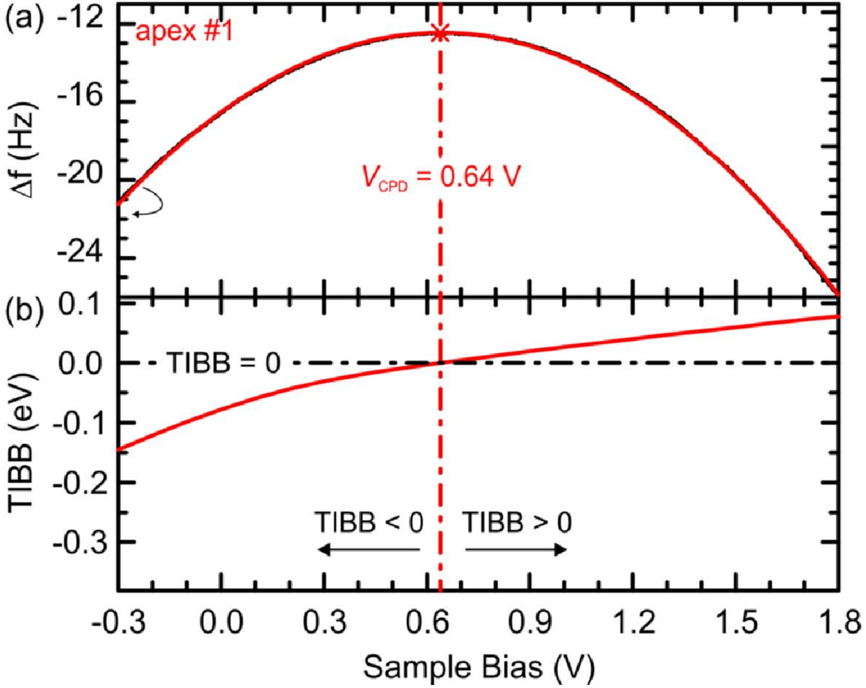
$$V_{Bias} = -CPD/e$$

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



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

G. Münnich, AD, J. Repp, and M. Wenderoth,
Phys. Rev. Lett **111**, 216802 (2013)



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

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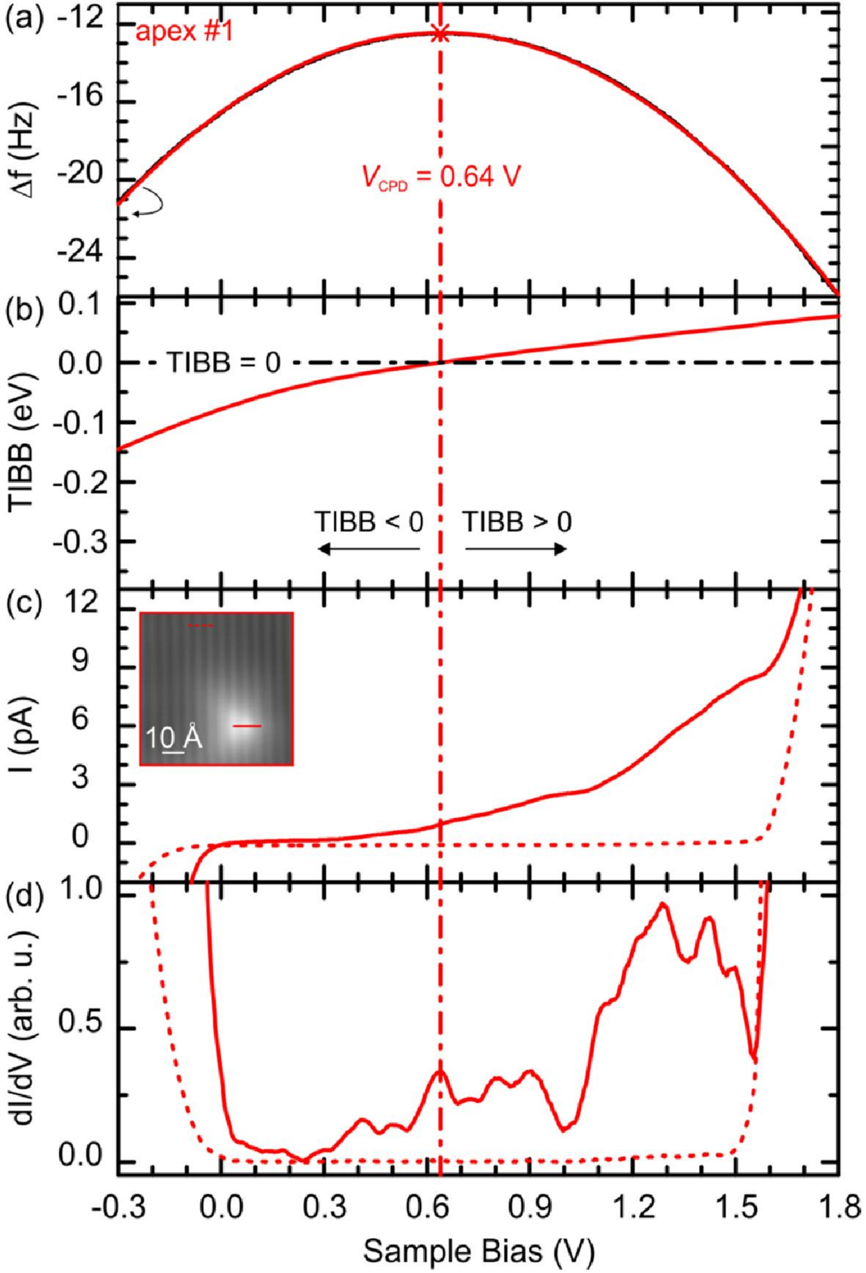

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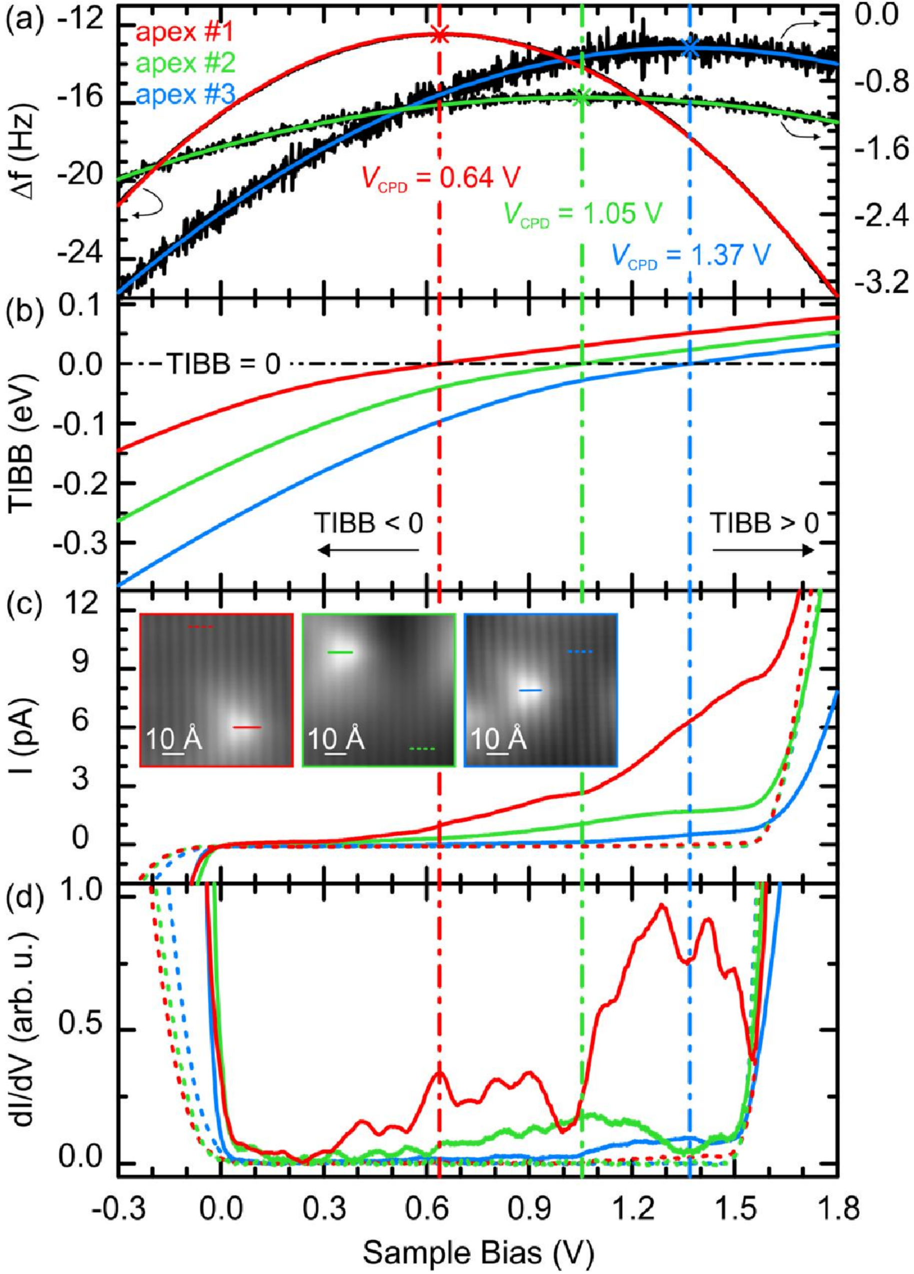
STM related to the flat-band voltage

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

G. Münnich, AD, J. Repp, and M. Wenderoth, *Phys. Rev. Lett* **111**, 216802 (2013)



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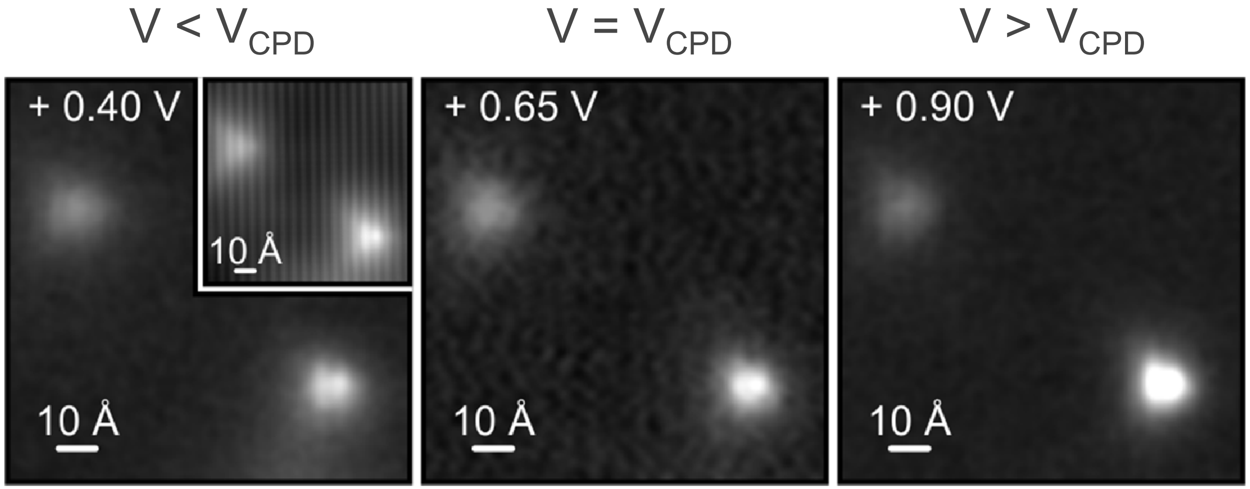
One and only mechanism

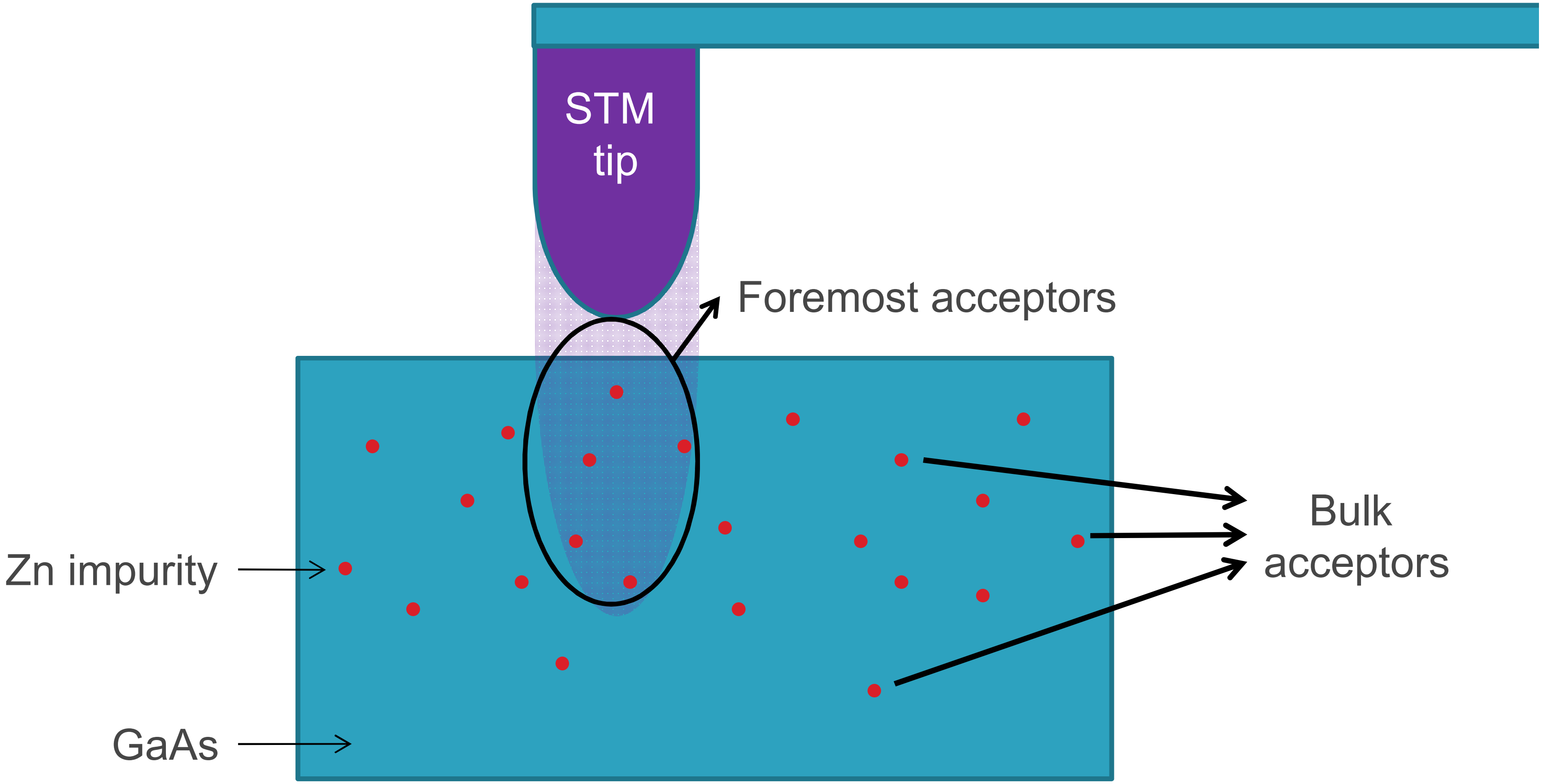


Constant-height dI/dV maps reveal a similar triangular feature of enhanced conductance in negative, zero and positive TIBB regimes

One conduction mechanism is active in all three band bending regimes

G. Münnich, A. Donarini, J. Repp, and M. Wenderoth, *Phys. Rev. Lett* **111**, 216802 (2013)

Model: Bulk vs. Foremost acceptors



The Hamiltonian for the junction

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

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

Geometry encoded

Anderson-Hubbard model

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

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

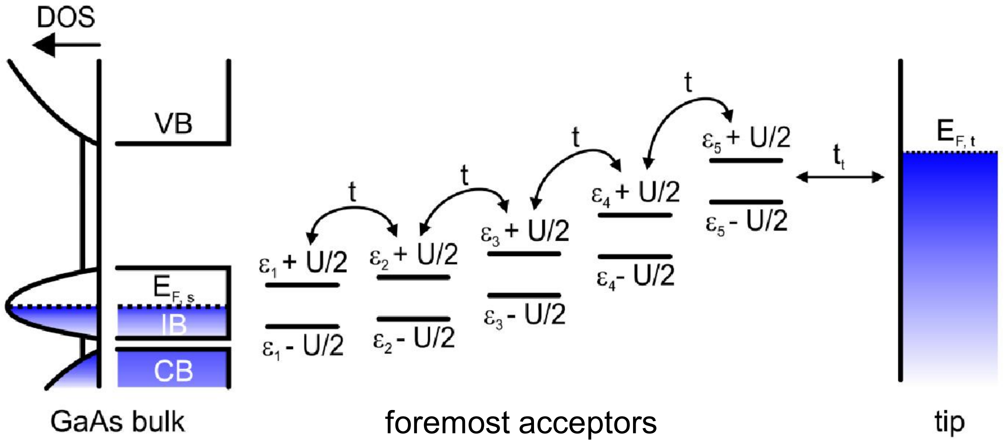
$$t = -5\mathrm{meV}$$

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

$$a_{\mathrm{B}} = 20\text{Å}$$

$$\varepsilon_r = 13$$

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



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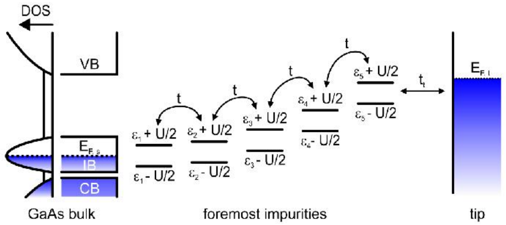
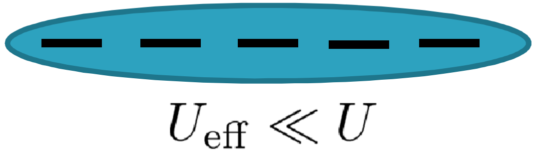
Anderson-Hubbard model

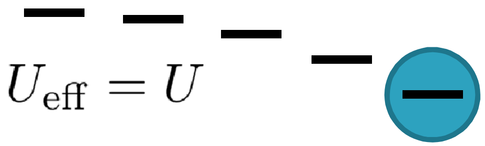


- We considered 5 acceptor states, giving a **Fock space** of dimension $4^5 = 1024$

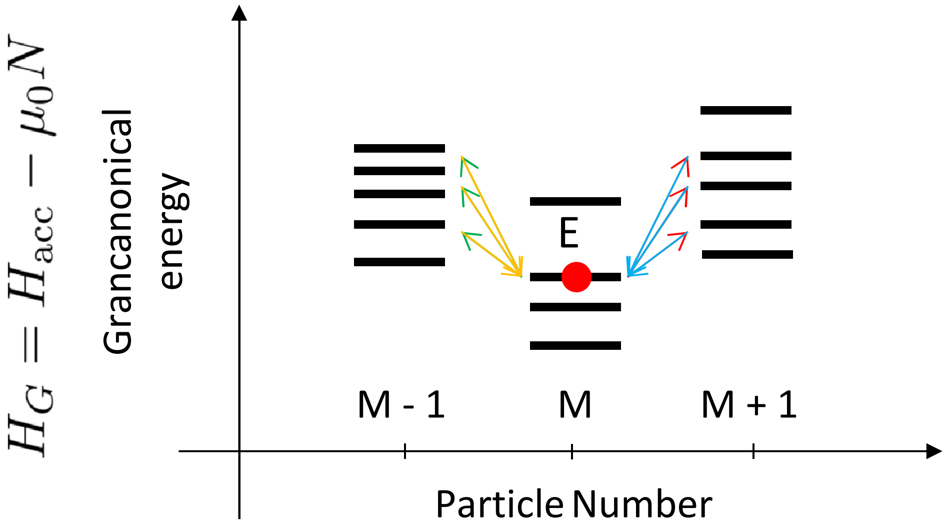
- In the flat band condition the system Hamiltonian is particle-hole symmetric
  - ➨ In absence of the tip: number of electrons = number of impurities
  - ➨ Constant terms in the interaction account for positive ions at the acceptor sites (**charge neutrality**)

- The addition energy of the Anderson-Hubbard Hamiltonian varies continuously with the bias: the model captures **crossover** between impurity band and the split off acceptor





Transport: master equation approach



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

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

Tunnelling rates

Bias dependent

The **many-body rates** read

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

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

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

Bias dependent

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

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

$$|t_S|^2/|t_T|^2 \approx 10^4$$ ← Extremly **asymmetric** coupling

Average current

- The average stationary current through the junction is calculated as:

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

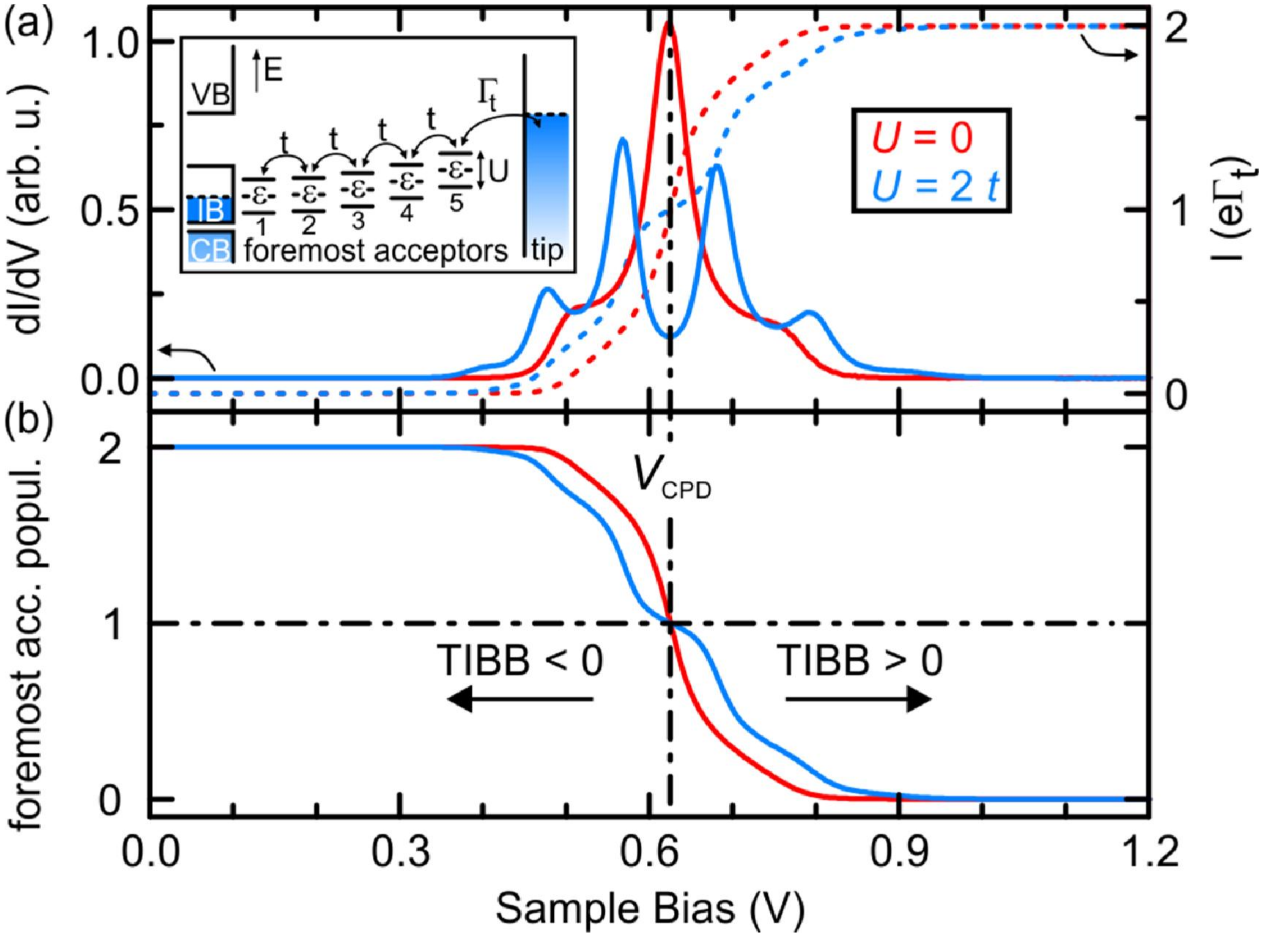
- In the limit of high bias ($V \approx V_{\mathrm{CPD}}$) and large asymmetry ($\Gamma^T \ll \Gamma^S$)

$$I_T = \sum_{\sigma ME} \Gamma^T_N \langle ME | d_{N\sigma} d^\dagger_{N\sigma} | ME \rangle P^{\mathrm{stat}}_{ME} = \Gamma^T_N (2 - \langle n_N \rangle)$$

$\uparrow$

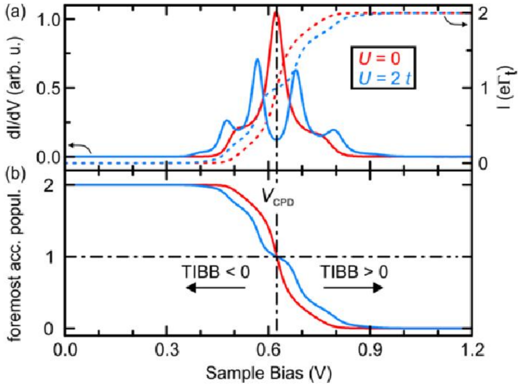
average occupation of the most superficial acceptor

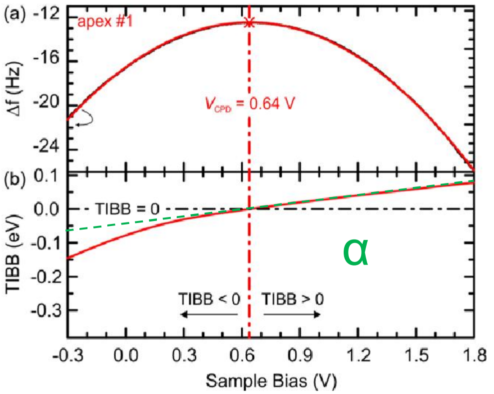
Current and differential conductance



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

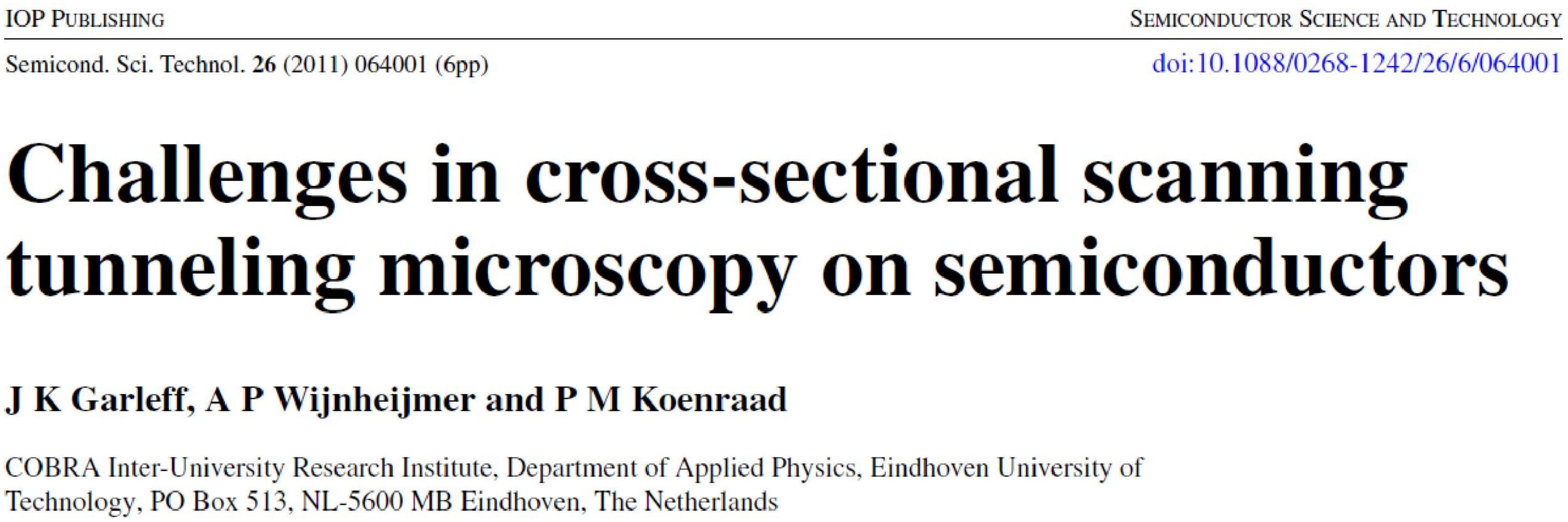




Conclusions

- Cross sectional STM on semiconductors is largely affected by **tip induced band bending** (TIBB)
- A combined **STM/KPFM** experiment fixes the flat band condition
- Current flows through **the same transport channel** in the 3 bending conditions.
- The Anderson-Hubbard model captures the **crossover** between **delocalized** state of the impurity band and **localized** split off impurity
- The current is determined by the **occupation of the last impurity**
- A rich variety of peak structures in the differential conductance indicates the **interplay** between the **tunnelling coupling** among the impurities and the **charging energy**

Thank you for your attention !



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

Challenges in cross-sectional scanning tunneling microscopy on semiconductors

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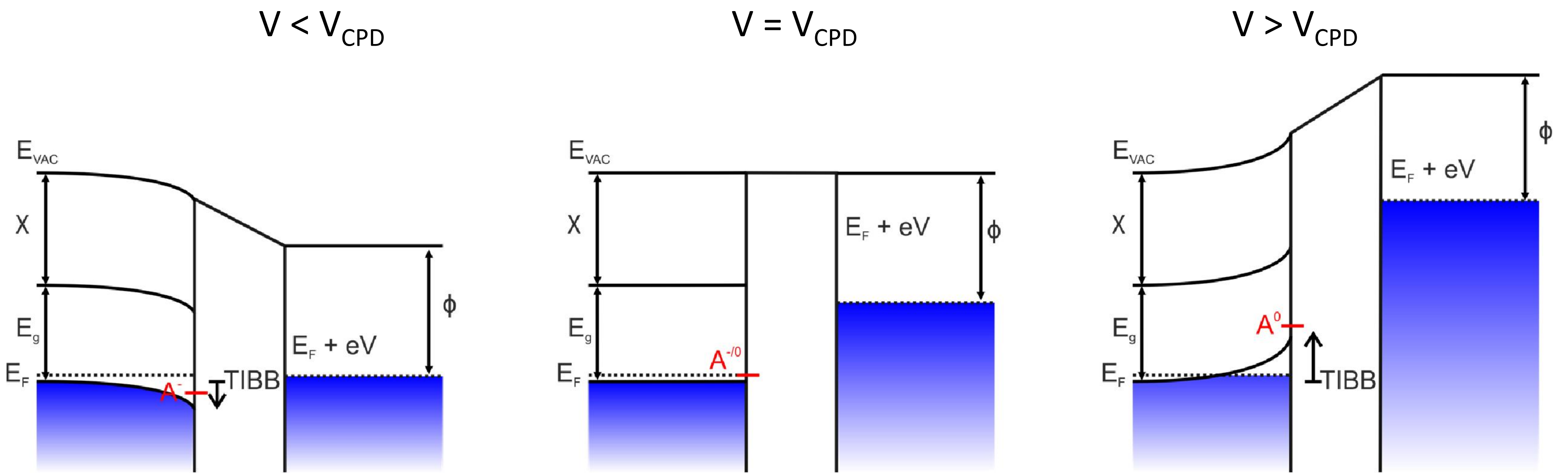
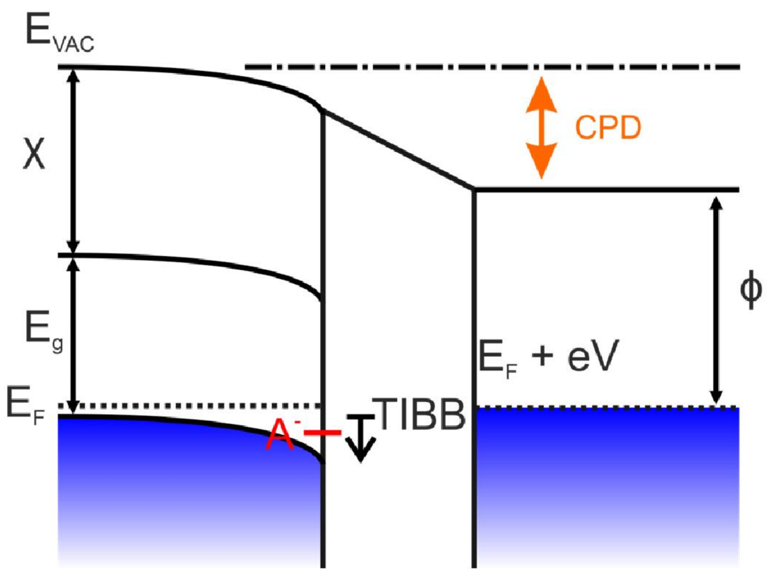
1. Cleavage
2. Surface properties affecting impurities
3. Tip impact - TIBB

Tip induced band bending (TIBB)



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

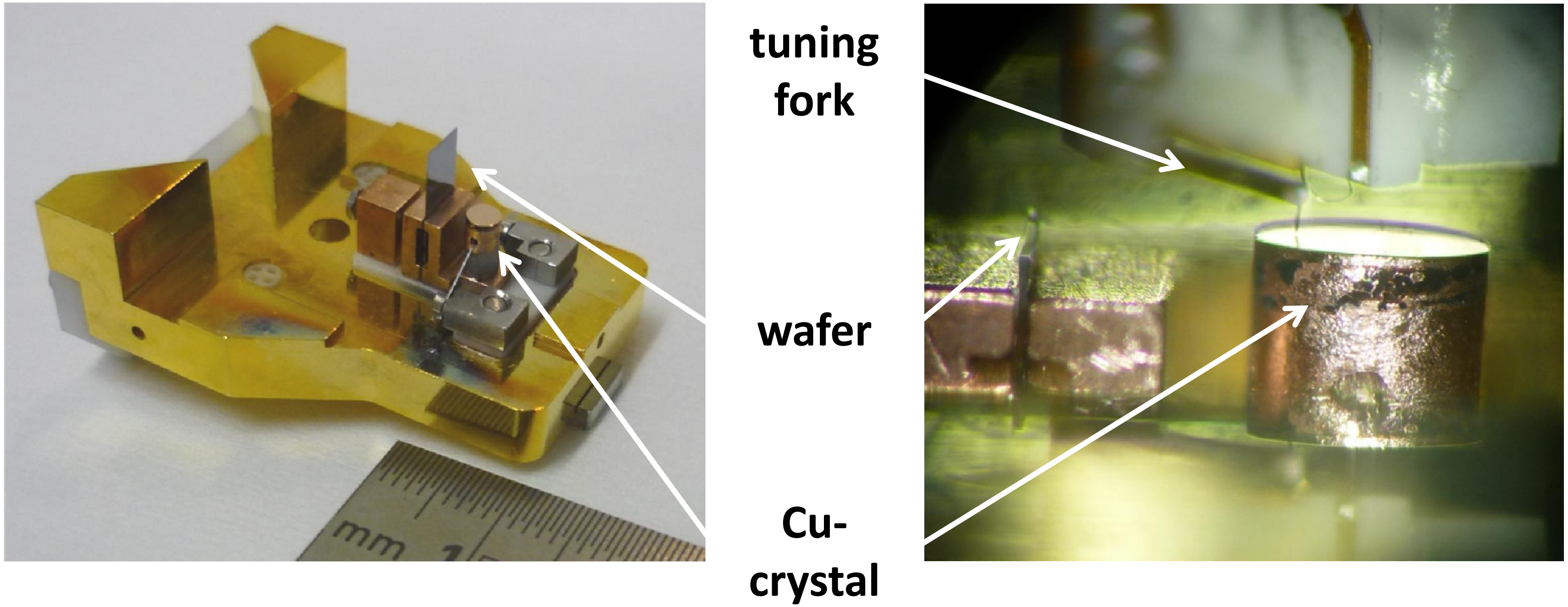
Tip induced band bending (TIBB)



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

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

Dual sample holder



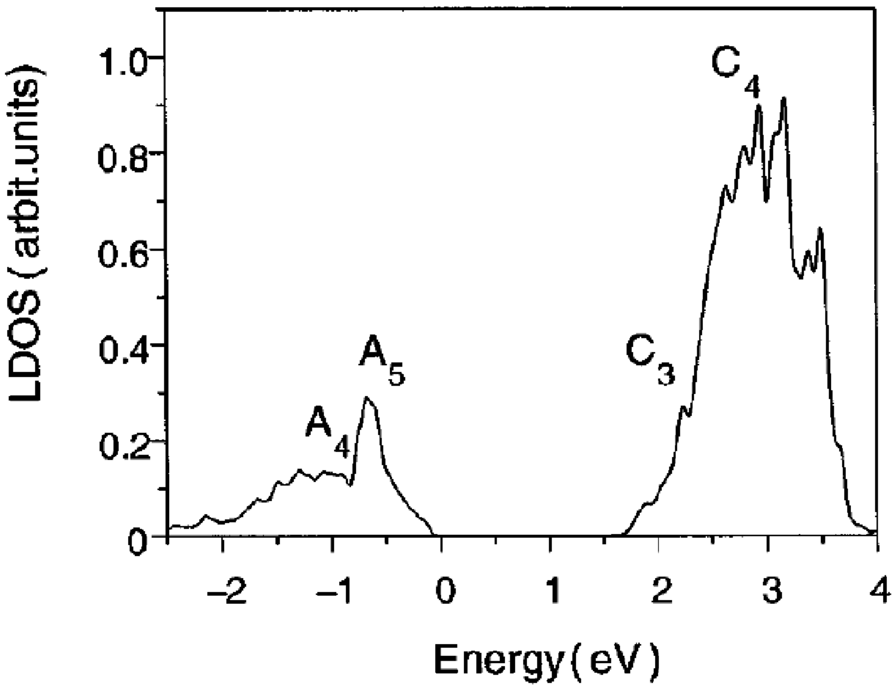
tuning fork

wafer

Cu-crystal

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

Electronic properties the GaAs(110) surface

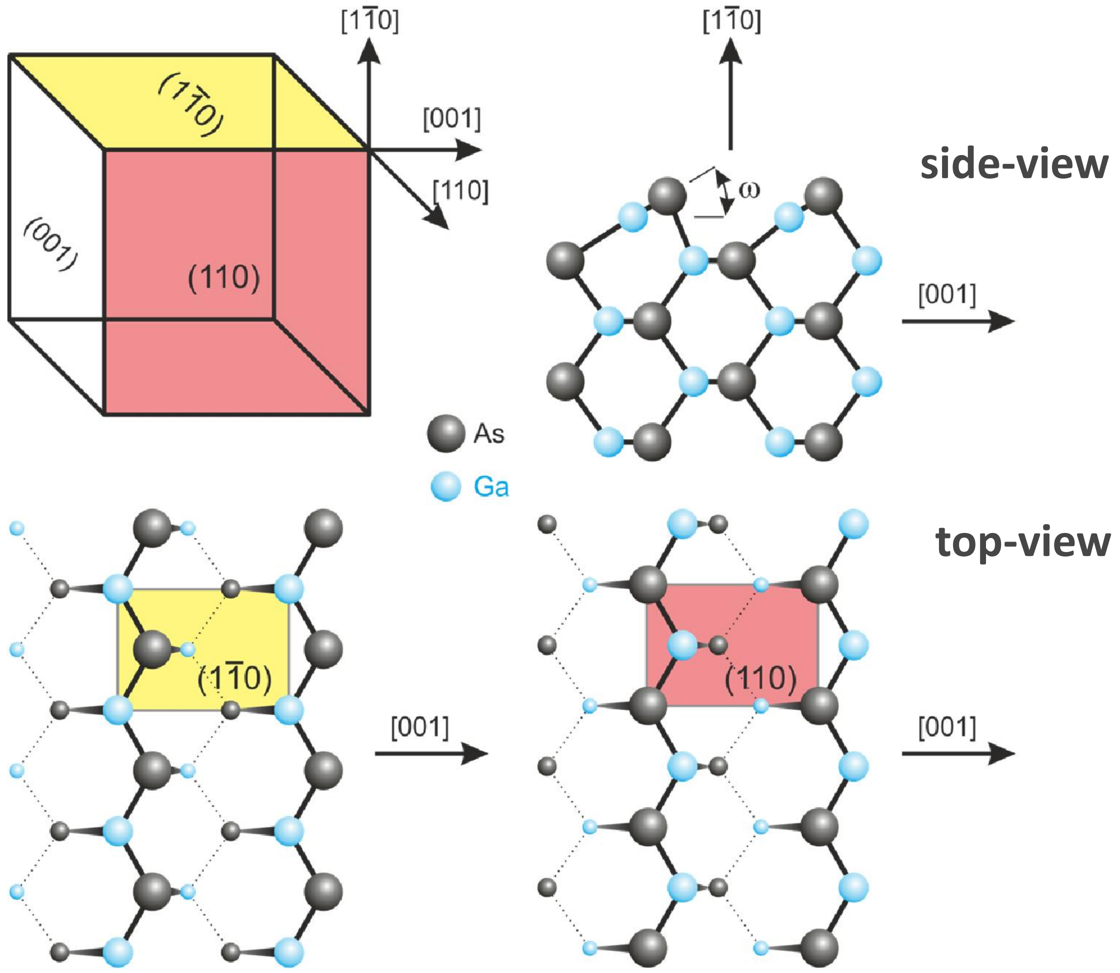


- 4 surface resonances outside the band gap

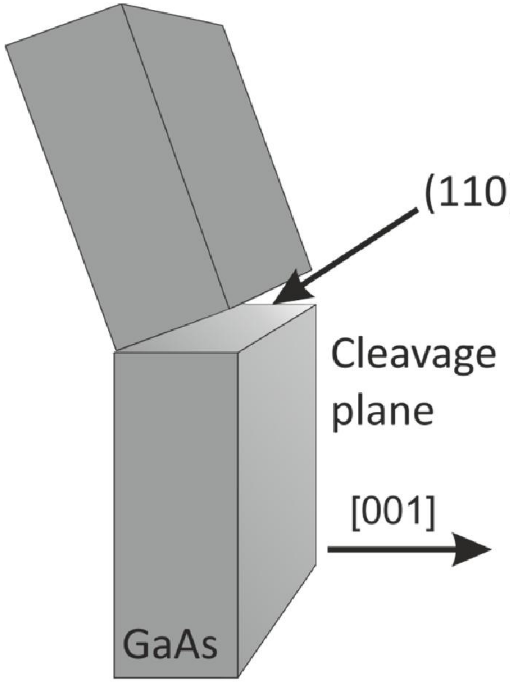
- Fermi-level not pinned:
  -> tunneling is only possible
     for certain bias voltages
  -> bulk DOS is not masked

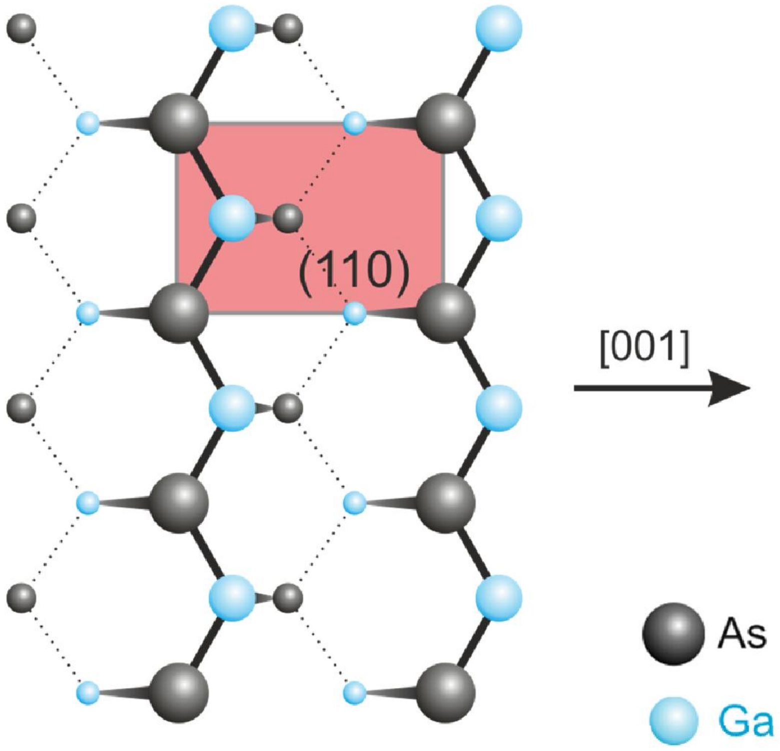
calculated DOS: Phys. Rev. Lett. **77**, 2997 (1995)

The {110} surfaces of GaAs



Crystallographic properties of GaAs



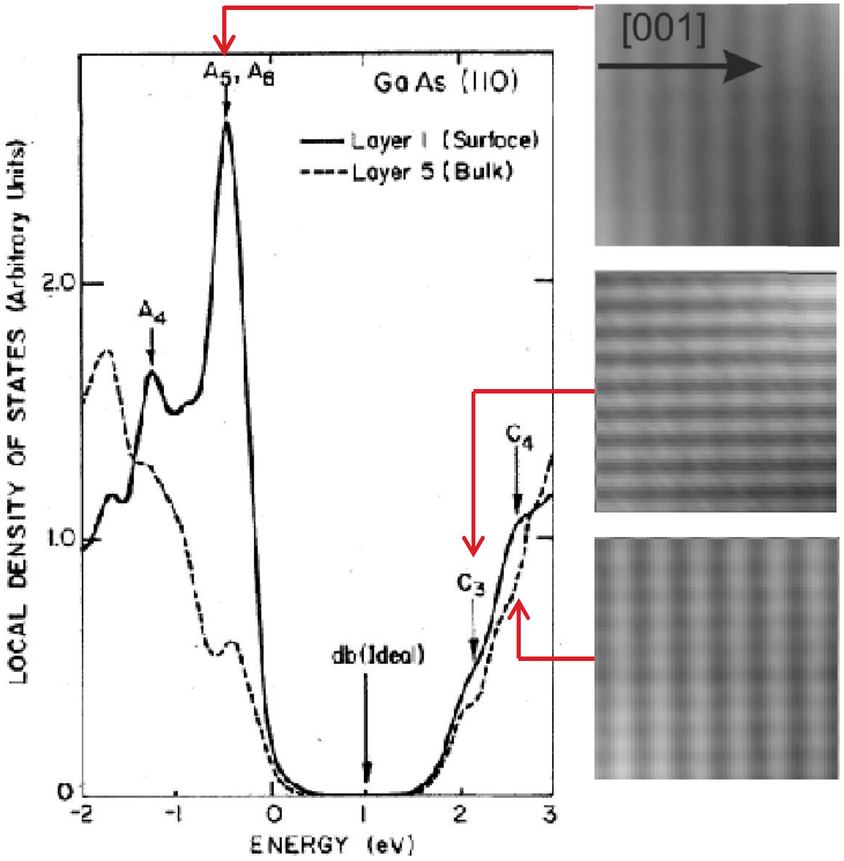


GaAs: III-V semiconductor, zinc-blende lattice structure.

(110) surface: prepared by cleaving of wafer, consists of alternating rows of As and Ga atoms

Sample System

Electronic properties of GaAs(110)



A5
U_{bias} = - 0.5 V

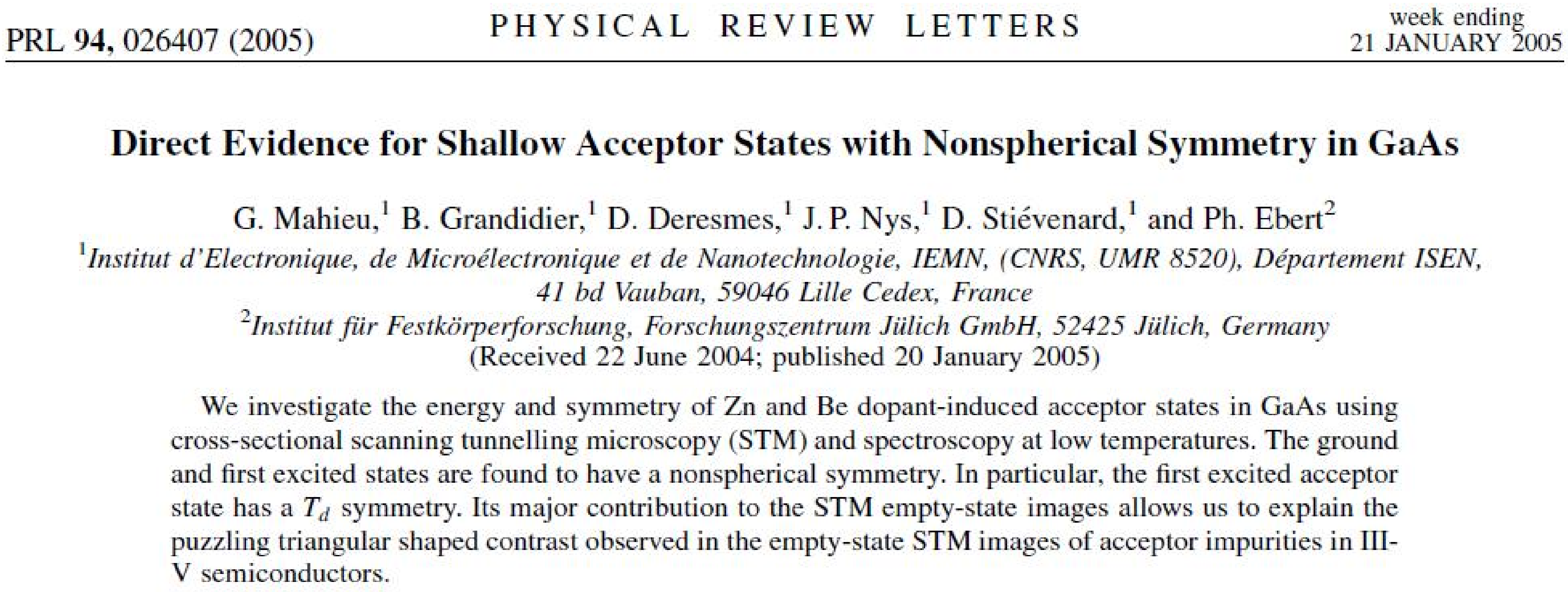
C3
U_{bias} = + 1.6 V

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]

Literature Review: Zn in GaAs



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

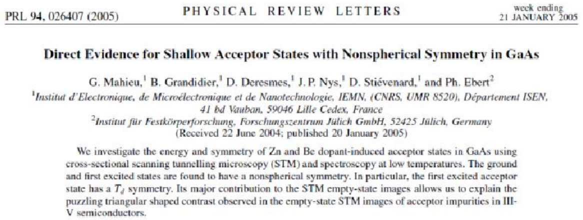
Direct Evidence for Shallow Acceptor States with Nonspherical Symmetry in GaAs

G. Mahieu,[1] B. Grandidier,[1] D. Deresmes,[1] J. P. Nys,[1] D. Stiévenard,[1] and Ph. Ebert[2]
[1]*Institut d'Electronique, de Microélectronique et de Nanotechnologie, IEMN, (CNRS, UMR 8520), Département ISEN, 41 bd Vauban, 59046 Lille Cedex, France*
[2]*Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany*

(Received 22 June 2004; published 20 January 2005)

We investigate the energy and symmetry of Zn and Be dopant-induced acceptor states in GaAs using cross-sectional scanning tunnelling microscopy (STM) and spectroscopy at low temperatures. The ground and first excited states are found to have a nonspherical symmetry. In particular, the first excited acceptor state has a T_d symmetry. Its major contribution to the STM empty-state images allows us to explain the puzzling triangular shaped contrast observed in the empty-state STM images of acceptor impurities in III-V semiconductors.

Literature Review: Zn in GaAs



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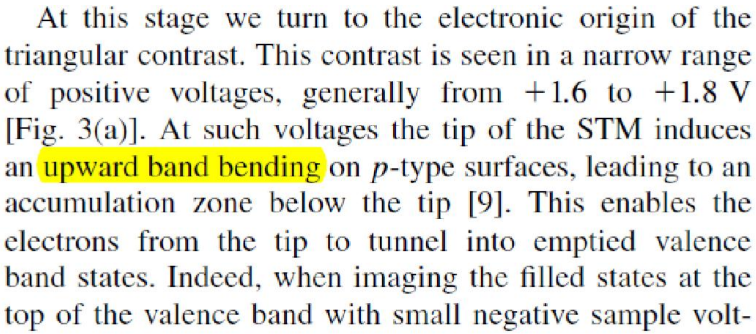
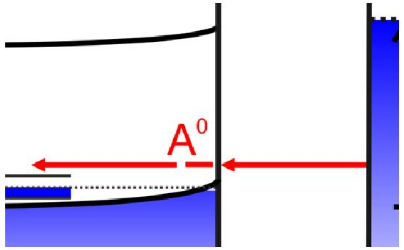
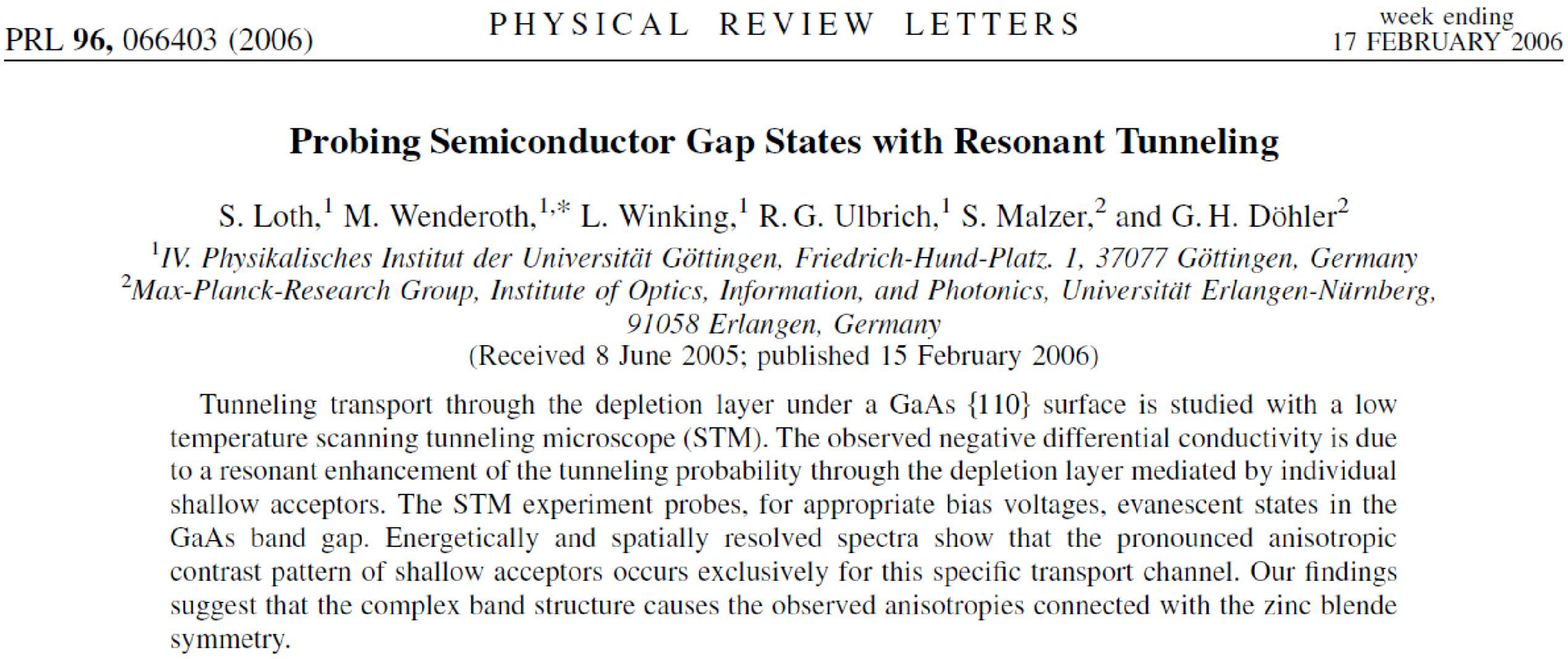


At this stage we turn to the electronic origin of the triangular contrast. This contrast is seen in a narrow range of positive voltages, generally from +1.6 to +1.8 V [Fig. 3(a)]. At such voltages the tip of the STM induces an upward band bending on p-type surfaces, leading to an accumulation zone below 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-



Literature Review: Zn in GaAs



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]
[1]*IV. Physikalisches Institut der Universität Göttingen, Friedrich-Hund-Platz. 1, 37077 Göttingen, Germany*
[2]*Max-Planck-Research Group, Institute of Optics, Information, and Photonics, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany*

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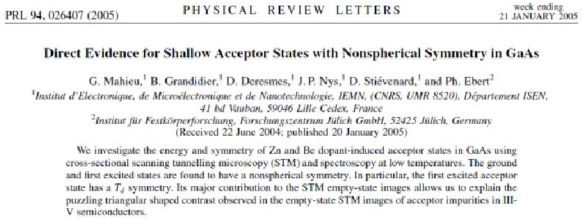
Tunneling transport through the depletion layer under a GaAs {110} surface is studied with a low temperature scanning tunneling microscope (STM). The observed negative differential conductivity is due to a resonant enhancement of the tunneling probability through the depletion layer mediated by individual shallow acceptors. The STM experiment probes, for appropriate bias voltages, evanescent states in the GaAs band gap. Energetically and spatially resolved spectra show that the pronounced anisotropic contrast pattern of shallow acceptors occurs exclusively for this specific transport channel. Our findings suggest that the complex band structure causes the observed anisotropies connected with the zinc blende symmetry.

Literature Review: Zn in GaAs



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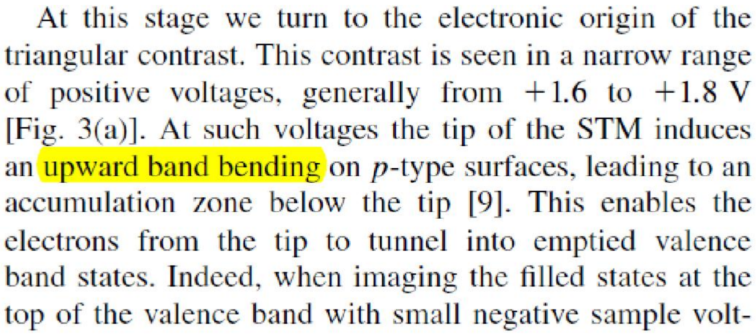

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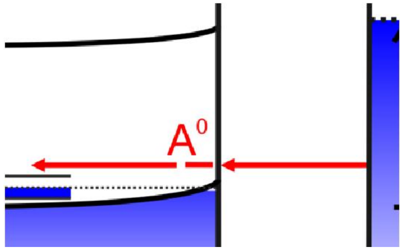

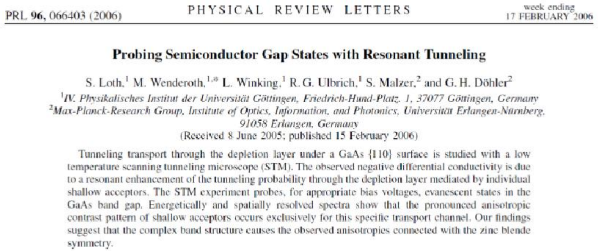

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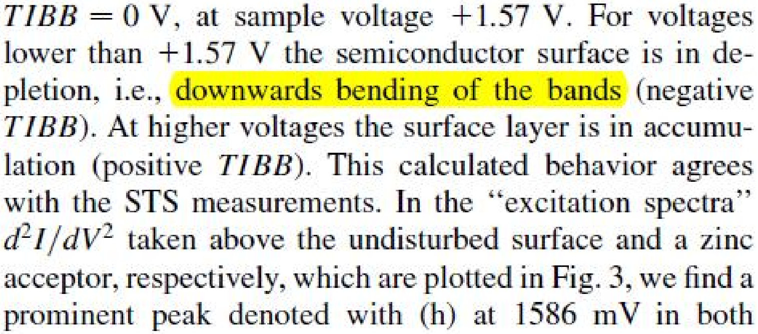
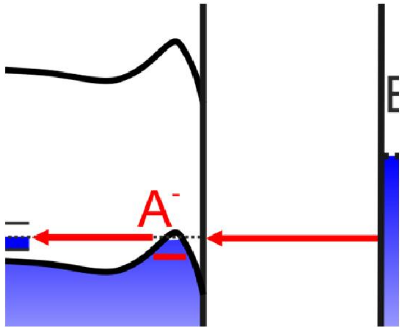
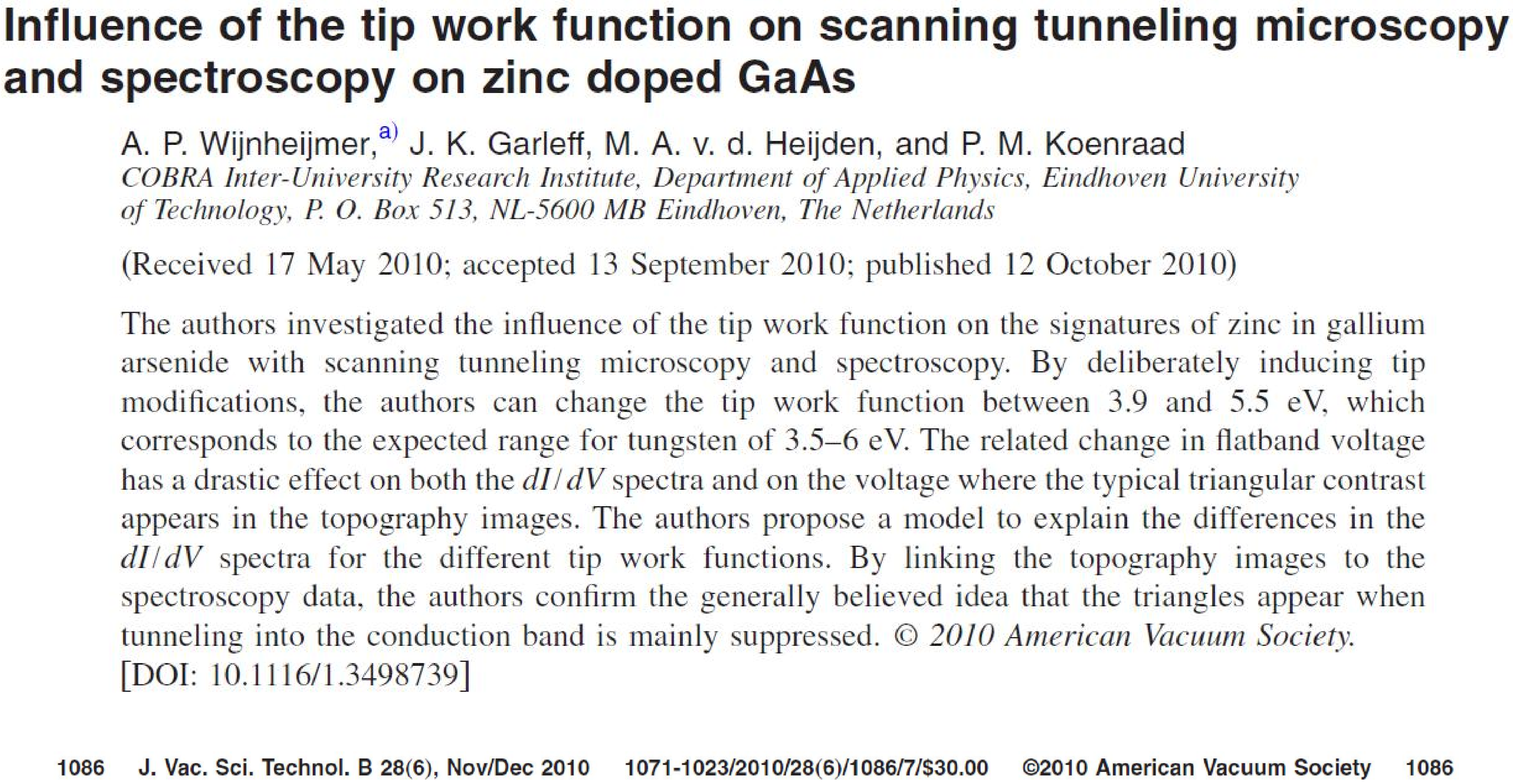


$TIBB = 0$ V, at sample voltage $+1.57$ V. For voltages lower than $+1.57$ V the semiconductor surface is in depletion, i.e., downwards bending of the bands (negative $TIBB$). At higher voltages the surface layer is in accumulation (positive $TIBB$). This calculated behavior agrees with the STS measurements. 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



Literature Review: Zn in GaAs



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
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(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]

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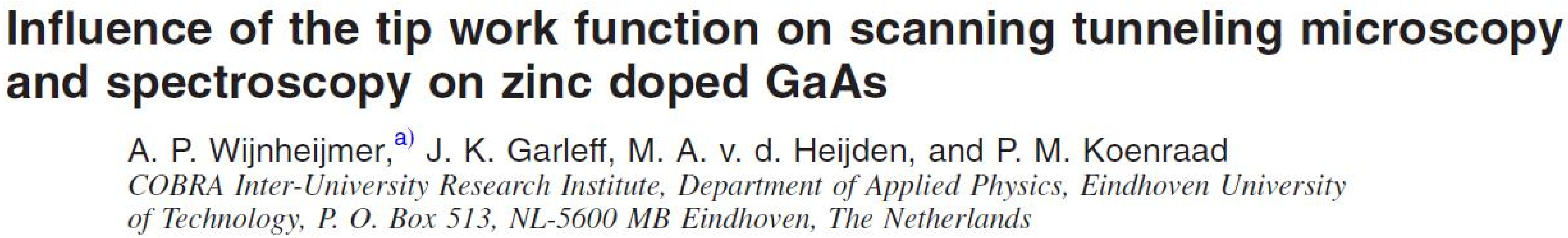
Literature Review: Zn in GaAs



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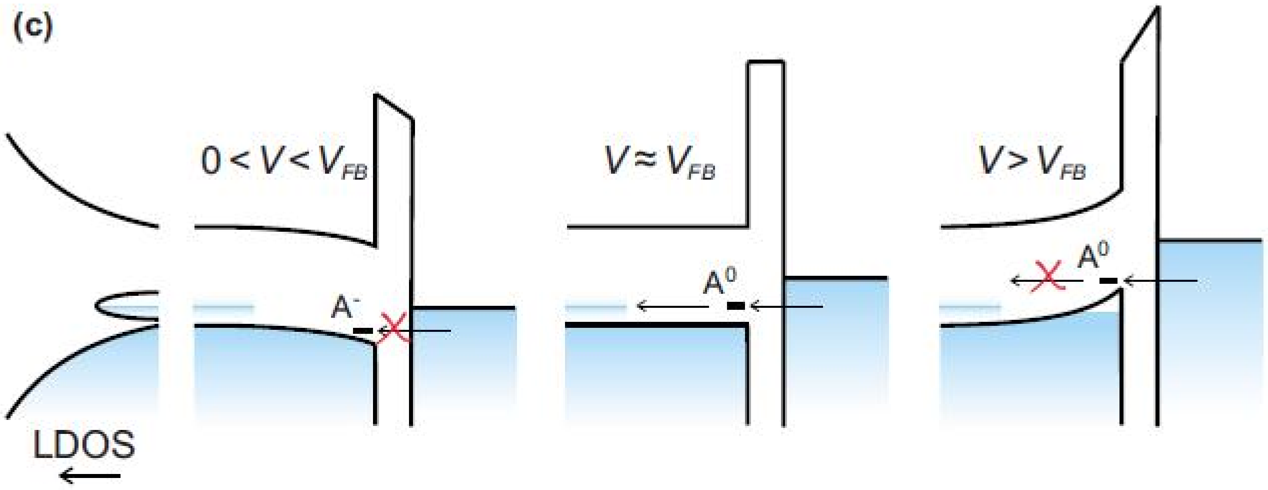

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Literature Review: Zn in GaAs - Summary

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

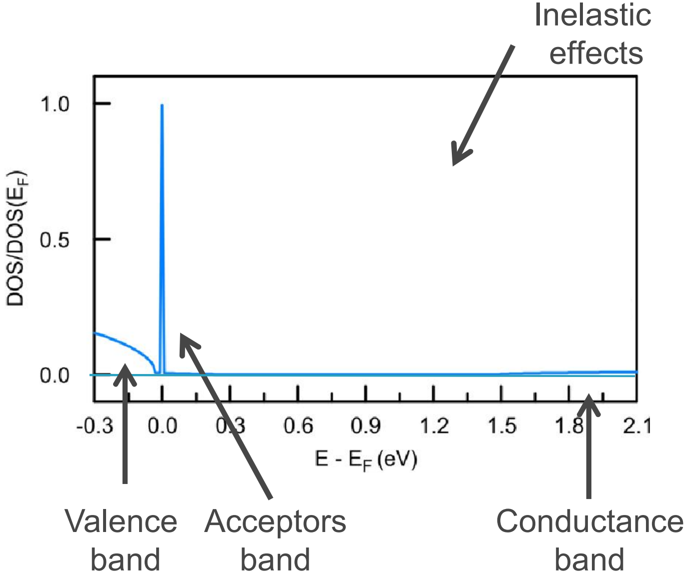
- All papers either guess the tip's work function or extract it from I(z), which is known to give only a rough estimate for Φ_{tip} (*J. Phys. Chem. C.* ***113****, 11301 (2009)*).

- The explanations given are based on single particle pictures of transport, or consider a single impurity.

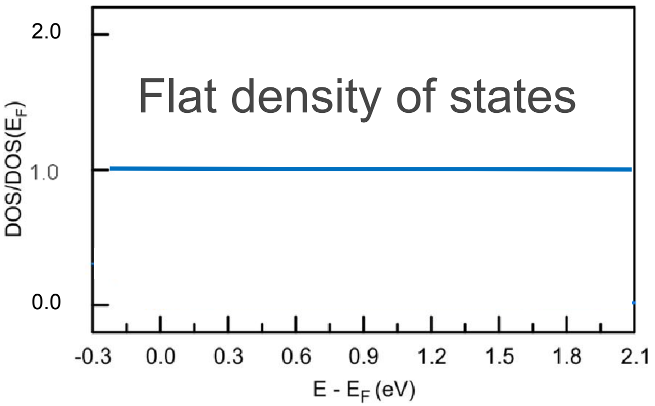
- Via combined X-STM/AFM, we have an exact method to determine the tip's work function: **Kelvin Probe Force Microscopy**

Leads modeling

Substrate



Tip

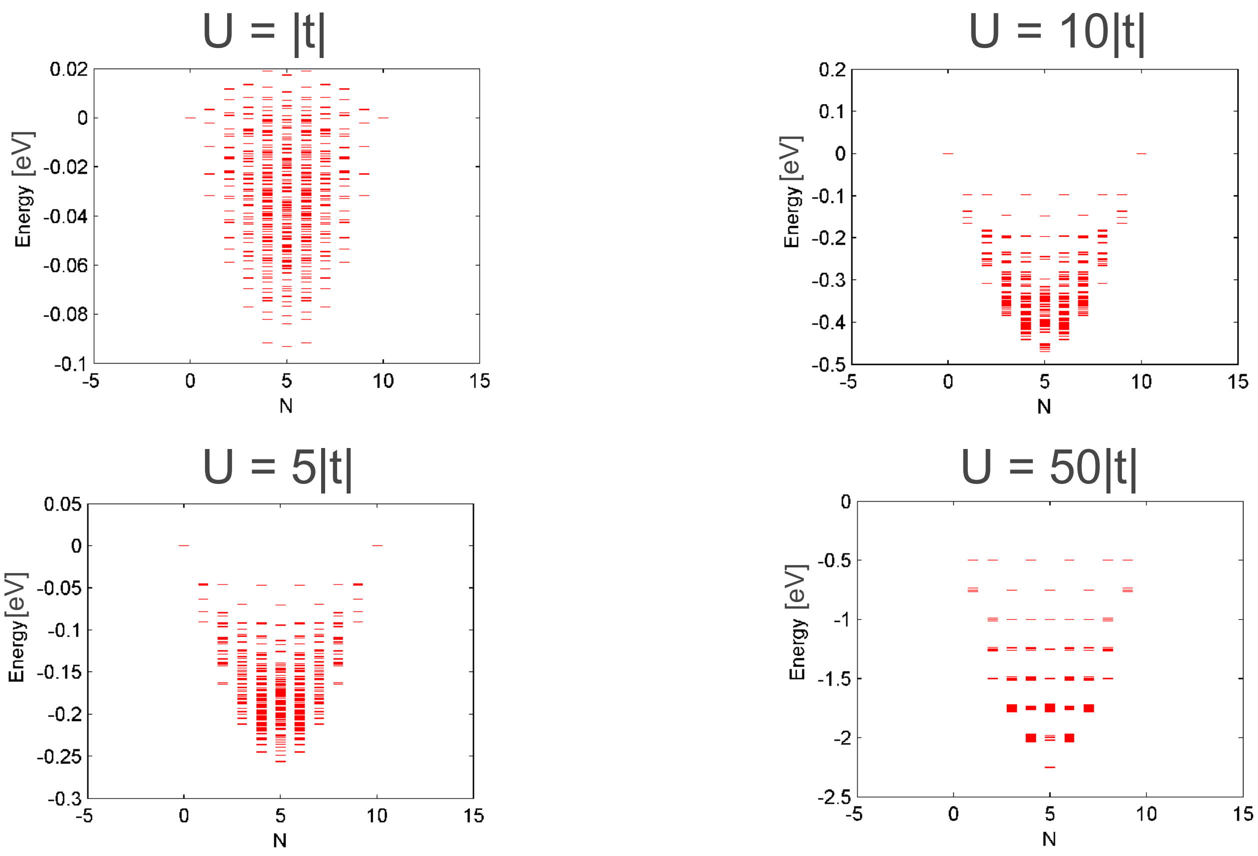


Free electron gas with:
Chemical potential μ_0
Temperture T

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

Spectrum of the Anderson-Hubbard Hamiltonians

t = -1 meV



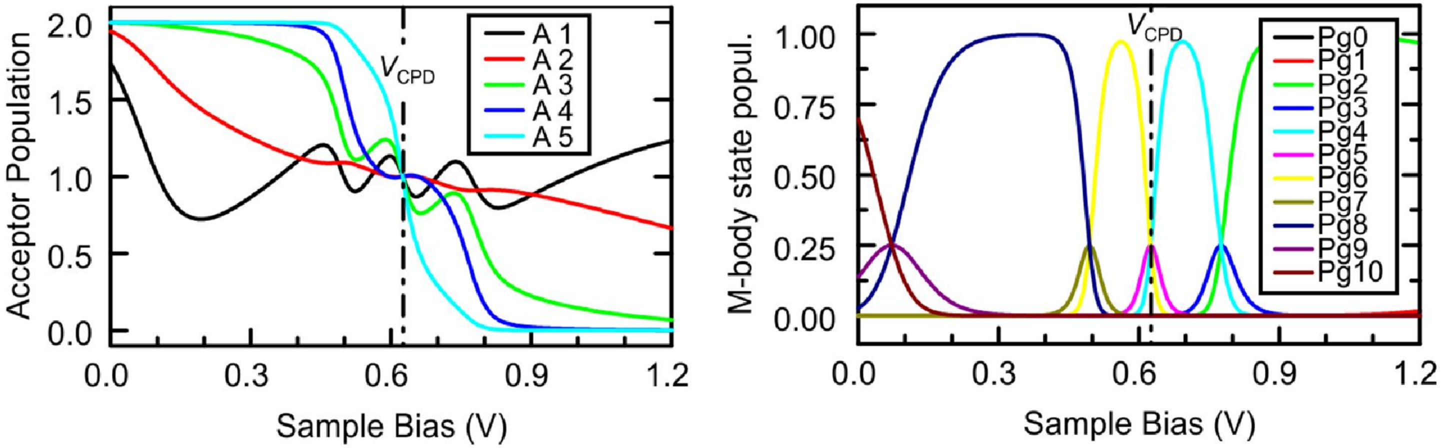
Particle-hole symmetry

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

Impurities occupations and many-body states populations

(a)

U = 0



U = 2 |t|

(b)