Artificial Atoms in Semiconductors

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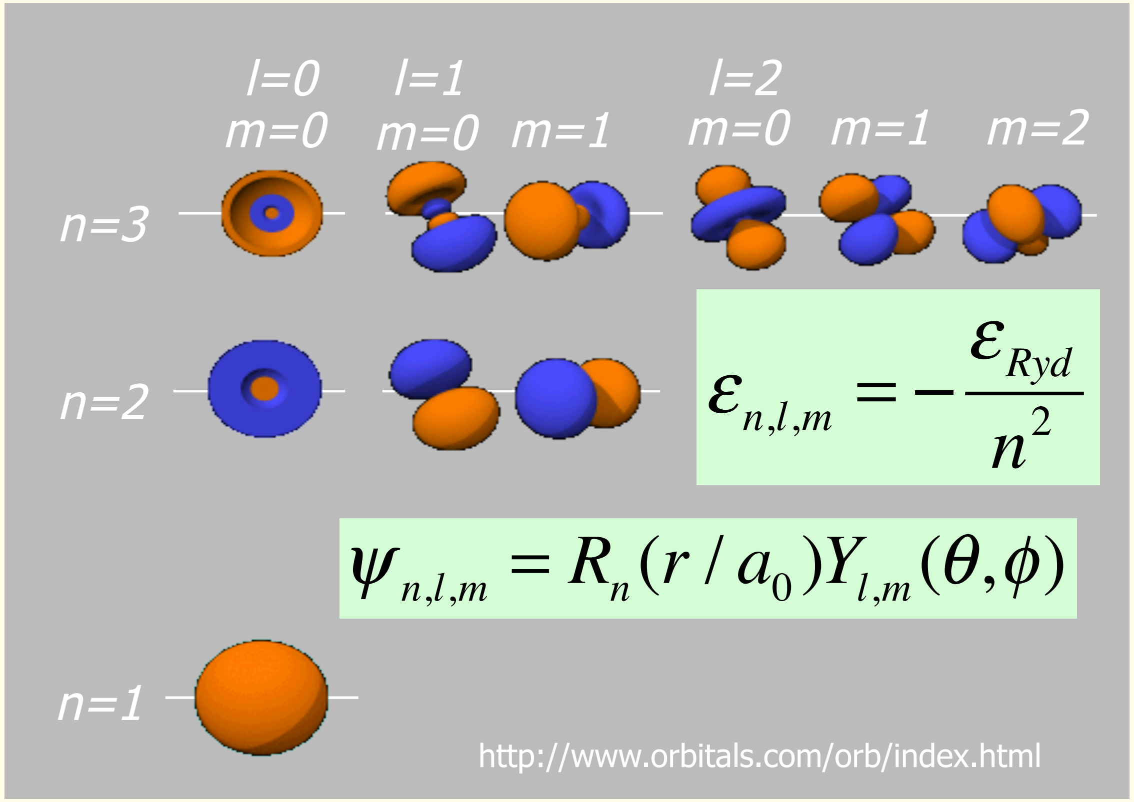
COBRA Inter-University Research Institute on Communication Technology

Atomic States Hydrogen

$$H\psi = \frac{\hbar^2 k^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi + \frac{1}{\varepsilon_o r}\psi = \varepsilon\psi$$



$$\varepsilon_{n,l,m} = -\frac{\varepsilon_{Ryd}}{n^2}$$

$$\psi_{n,l,m} = R_n(r/a_0)Y_{l,m}(\theta,\phi)$$

Rydberg energy

$$\varepsilon_{Ryd} = -\frac{me^4}{8h^2\varepsilon_o^2} = -13.6\ eV$$

Bohr radius

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2} = 0.053\ nm$$

Hydrogenic Impurity in a Semiconductor

Ground state wavefunction

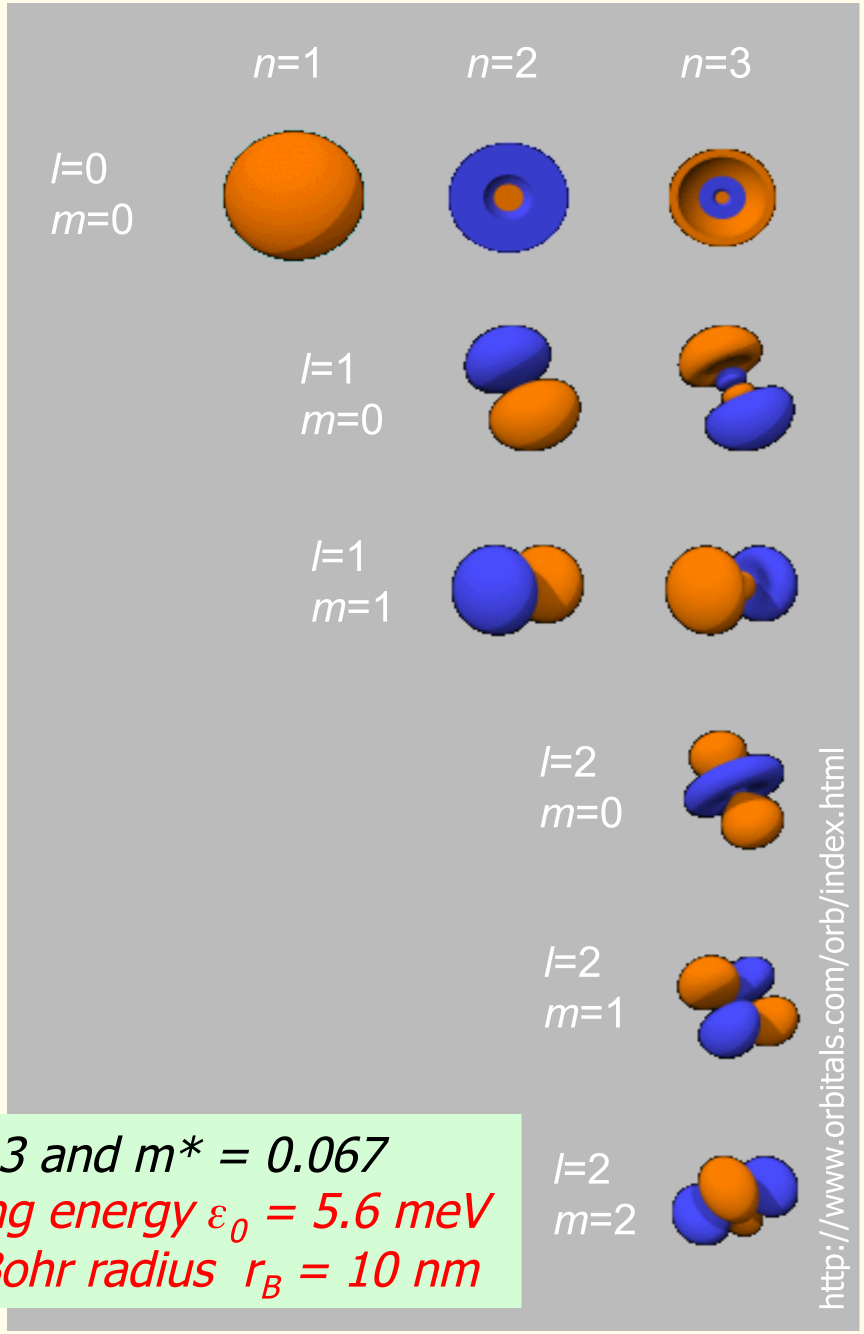
$$\psi(1s_{1/2}) = 2/\sqrt{4\pi}\left(1/r_B\right)^{3/2} e^{-r/r_B}$$

Effective Bohr-radius

$$r_B = \frac{\varepsilon_r}{m^*} a_0$$

Ground state binding energy

$$\varepsilon = \frac{m^*}{\varepsilon_r^{\,2}} \varepsilon_{Ryd}$$



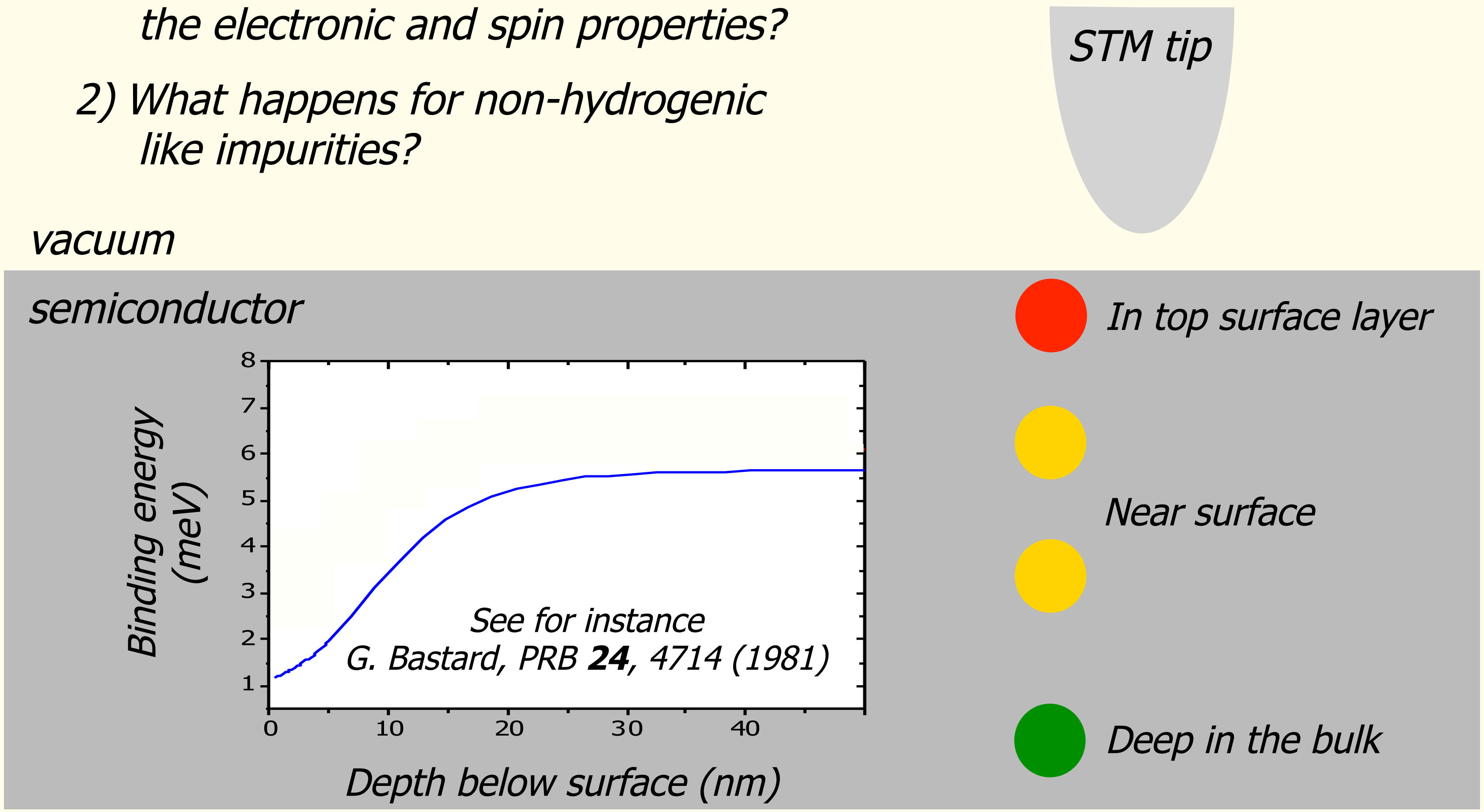
In GaAs ε_r = 13 and m = 0.067*
ground state binding energy ε_0 = 5.6 meV
and the effective Bohr radius r_B = 10 nm

Hydrogenic Atoms in Semiconductors

Questions:

1) what is the effect of the surface on the electronic and spin properties?

2) What happens for non-hydrogenic like impurities?



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Outline

- ✓*Introduction*
- ✓*Analysis of individual donors in GaAs*
  - ✓*Charge manipulation (ionization)*
  - ✓*Electronic characterization*
  - ✓*Configuration manipulation (donor/acceptor)*
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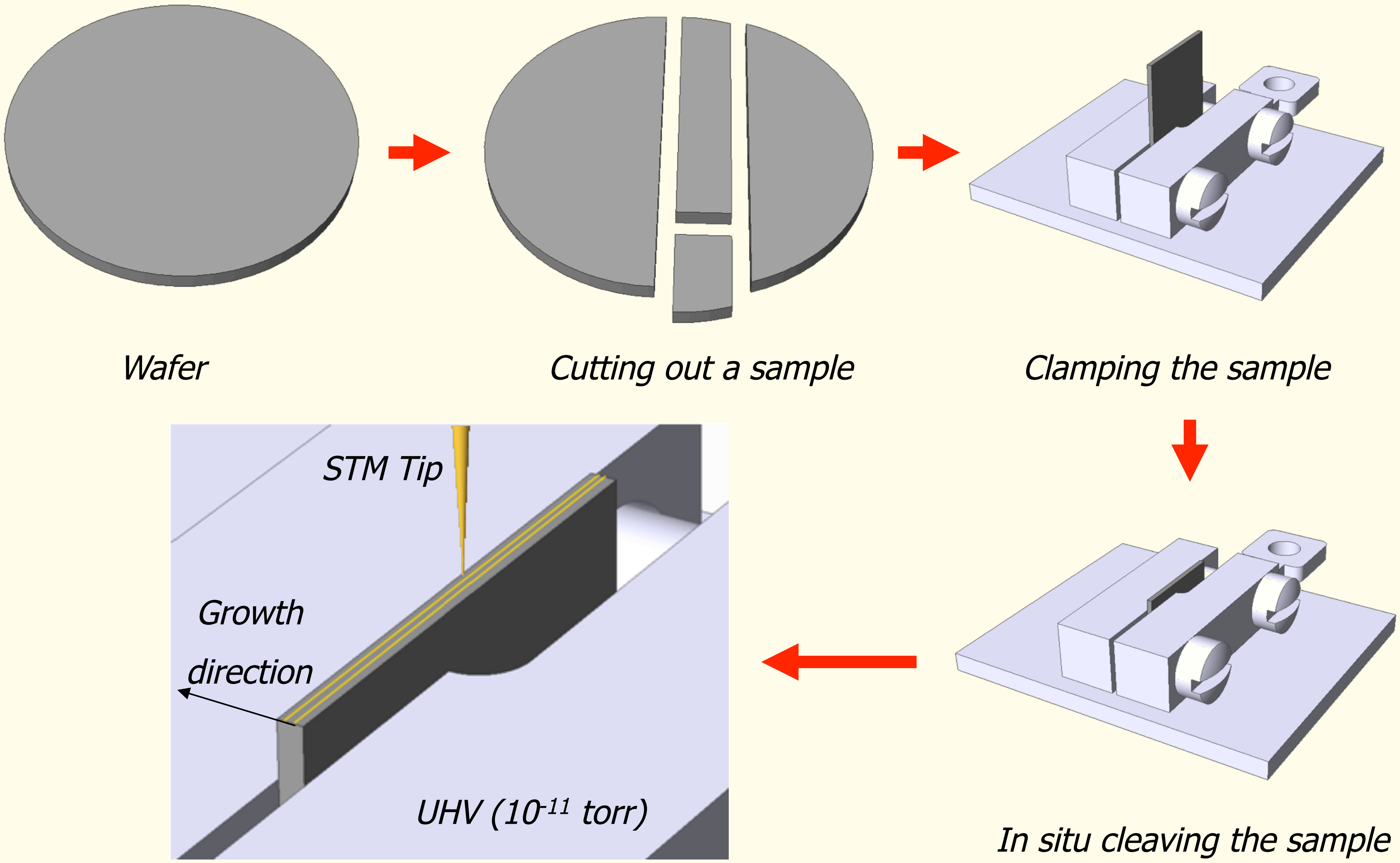
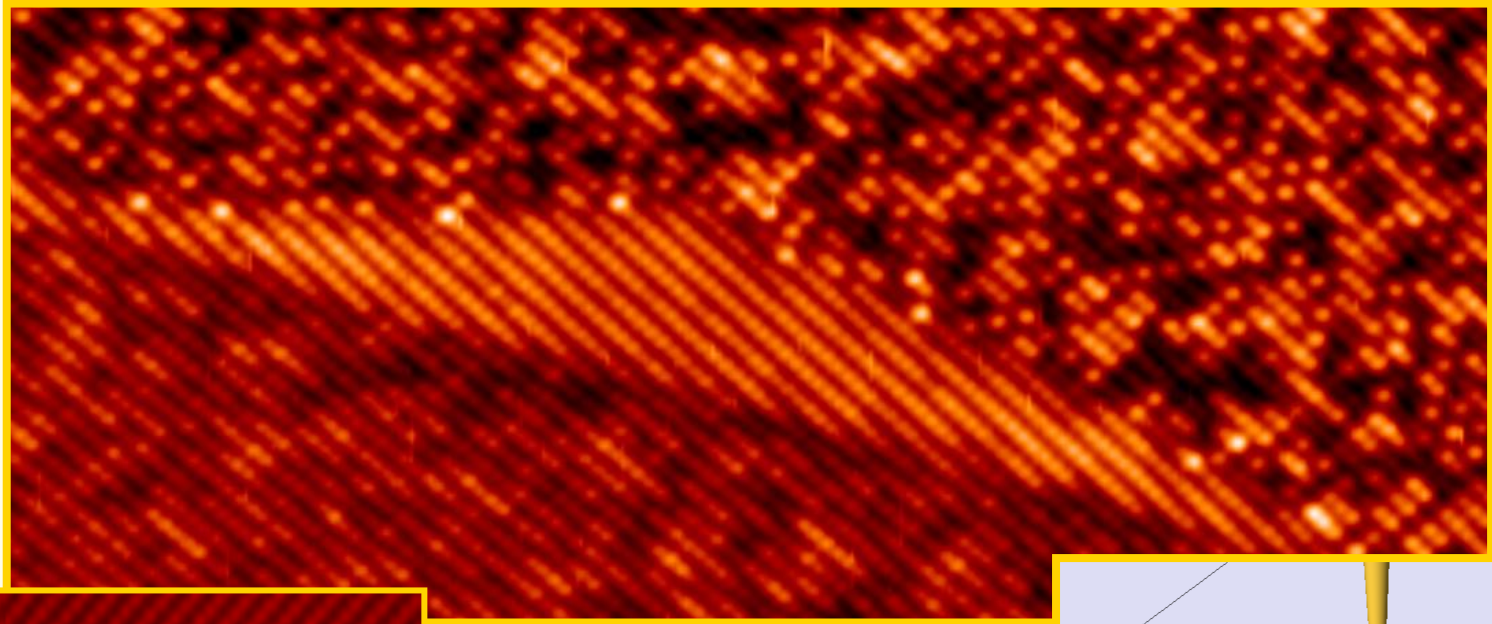
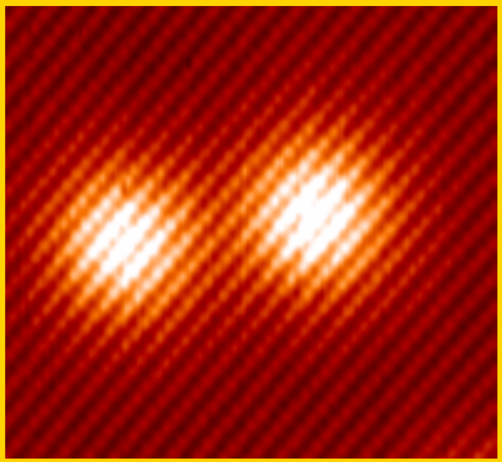
Cross-sectional STM



Assessment at the Atomic Scale

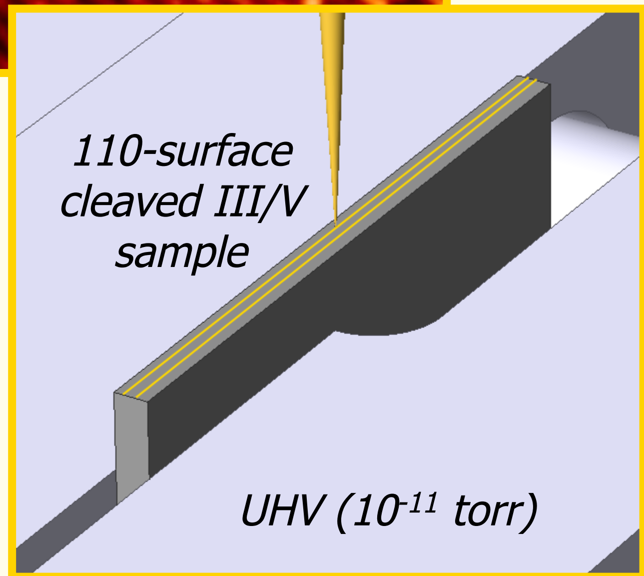


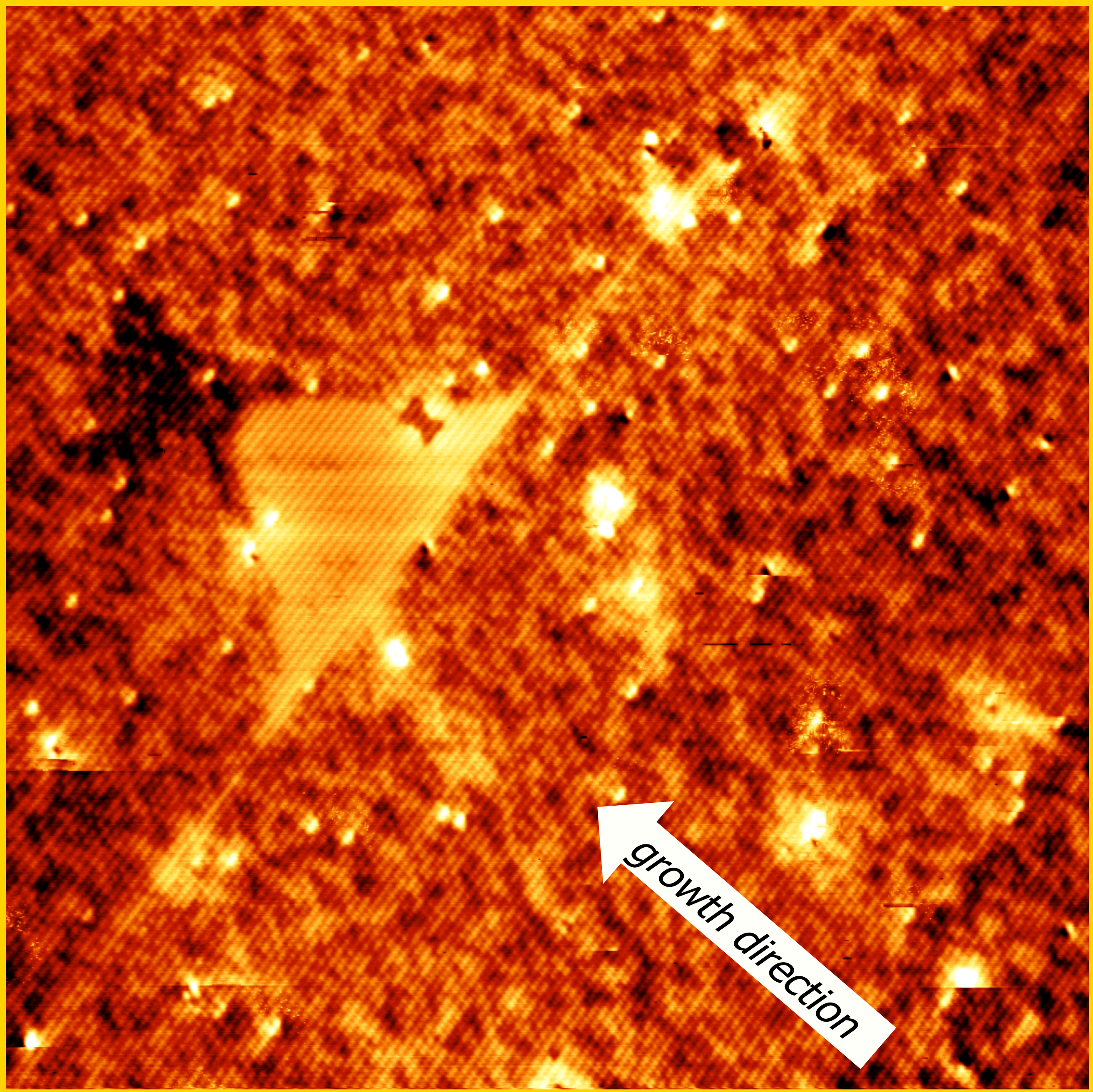
InAs self-assembled quantum dot in InGaAs



9 nm * 8 nm

Two Si impurities in GaAs



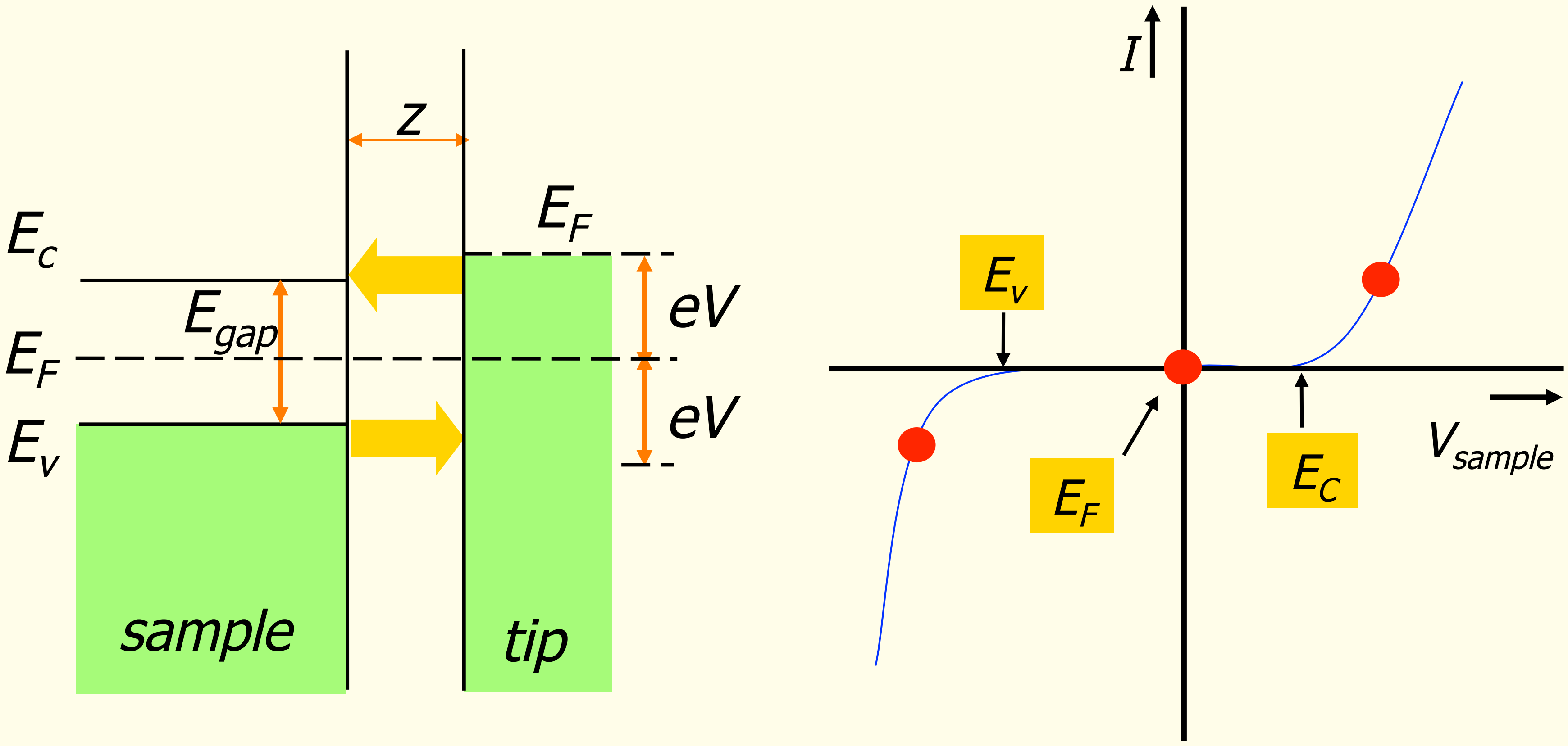


GaAs dot in AlGaAs grown by Ga droplet technique

Grown by T. Mano, Tsukuba, Japan

J.G.Keizer, J.G. et al, APL ***96****, 062101 (2010).*

Scanning Tunneling Microscopy on Semiconductors



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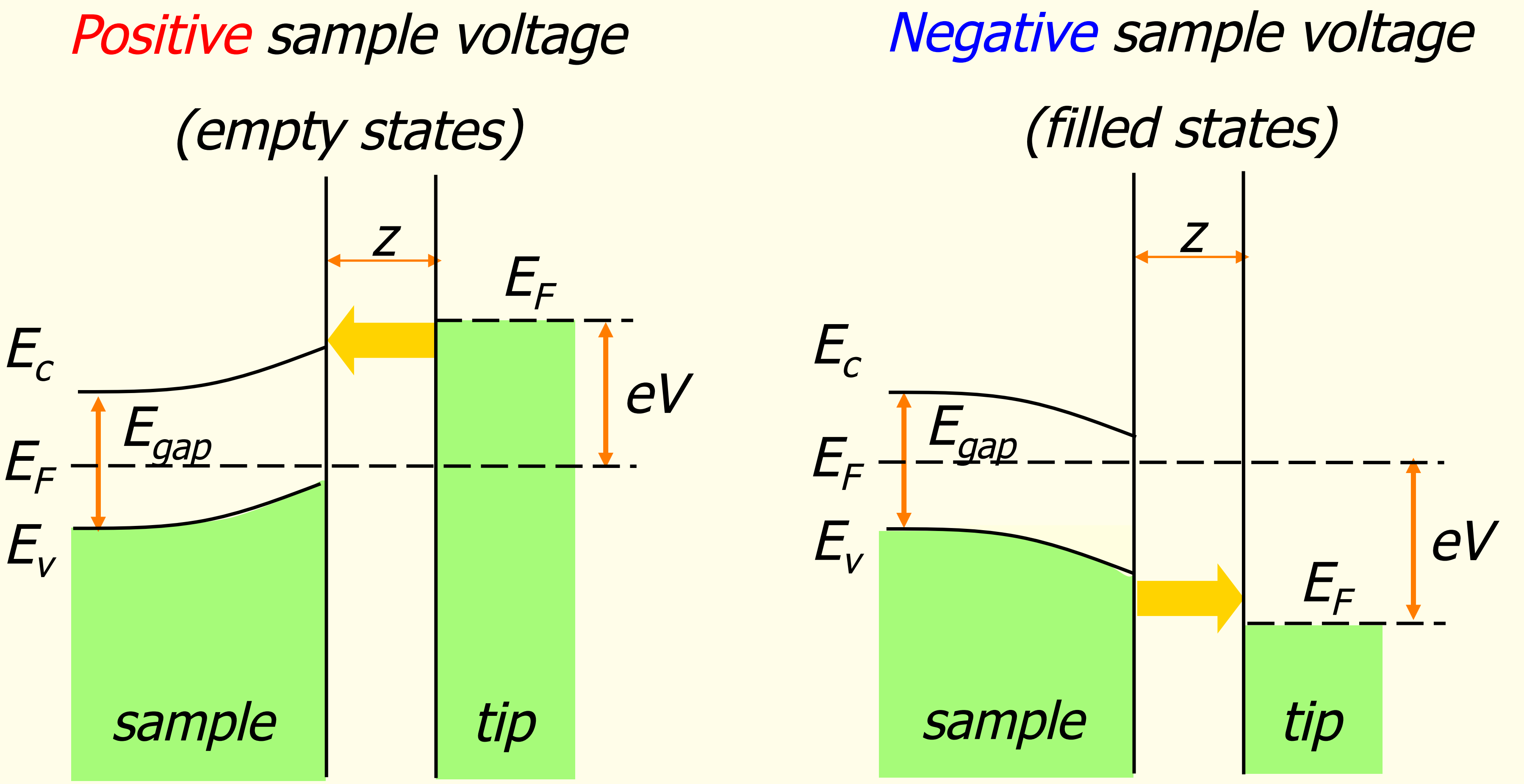
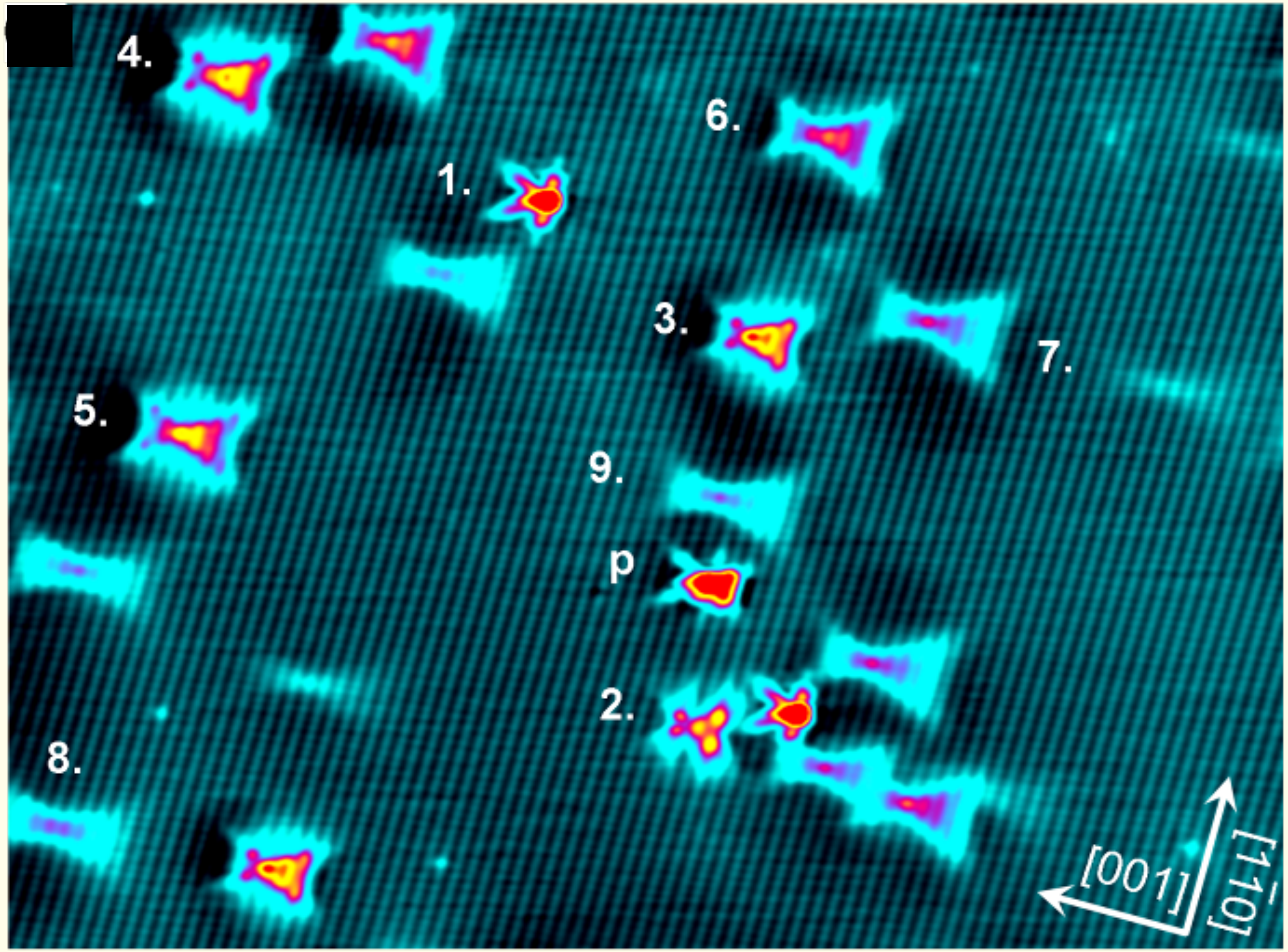


Depletion, accumulation, inversion

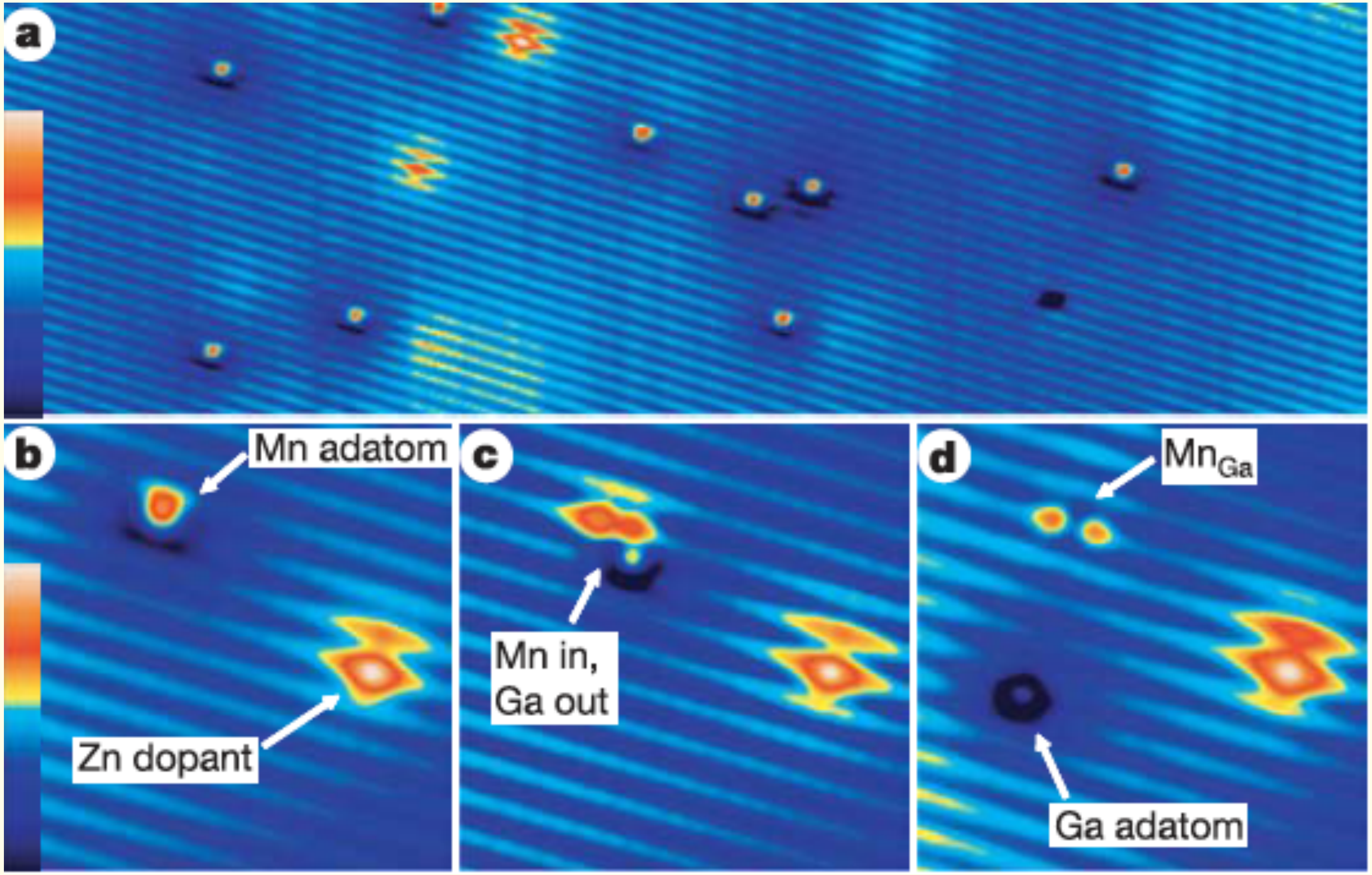
Bulk doped Mn:GaAs



*45 nm * 35 nm*

Celebi et al PRL ***104****, 086404 (2010)*

Mn Substitution in a GaAs Surface



*D. Kitchen et al, Nature **442**, 436 (2006)*

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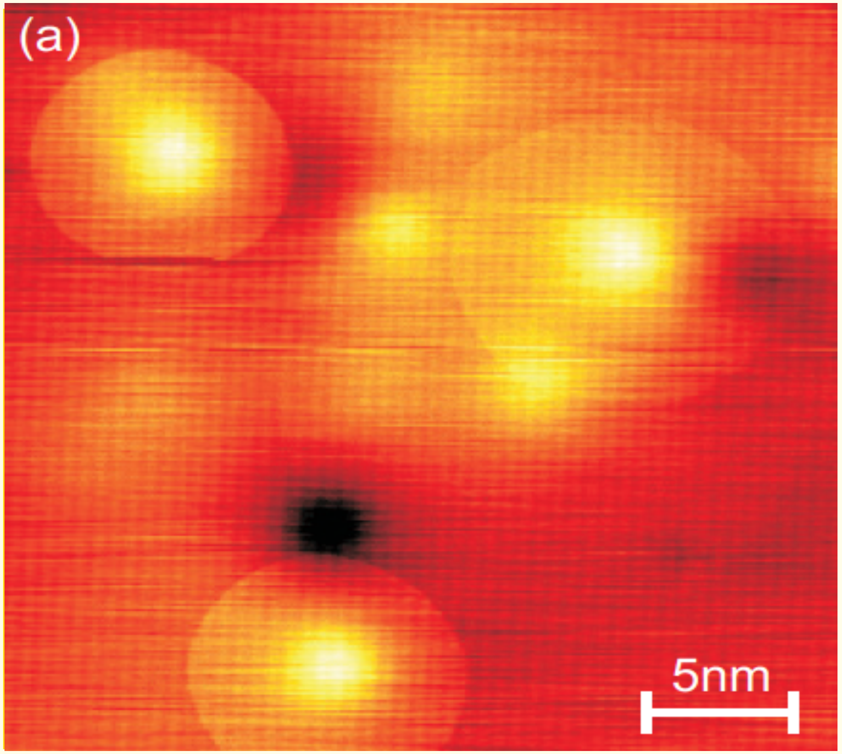
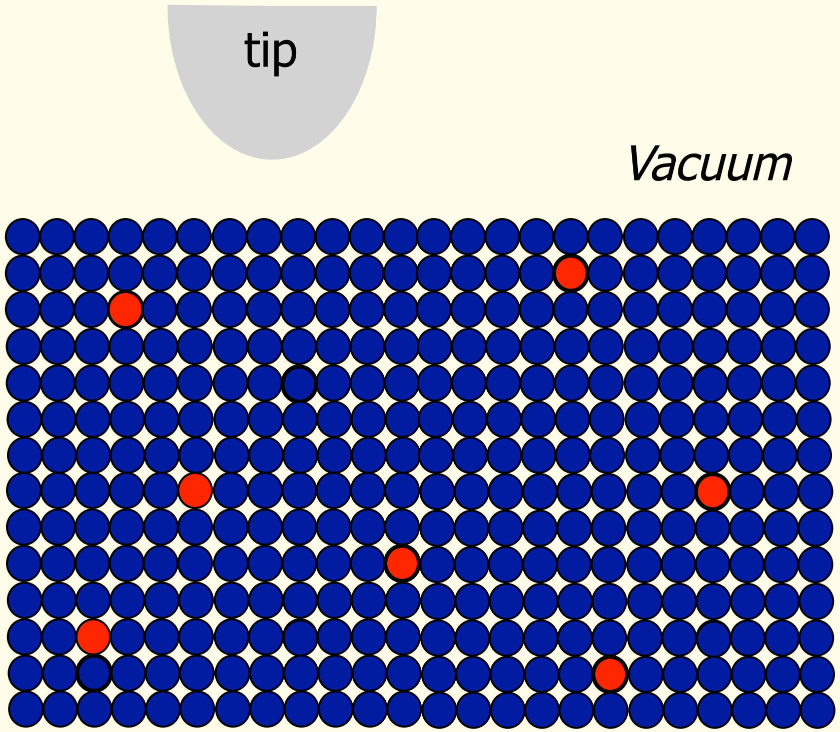
Low Temperature Imaging

Si Doped GaAs measured at 5 K



*50 nm * 50 nm*

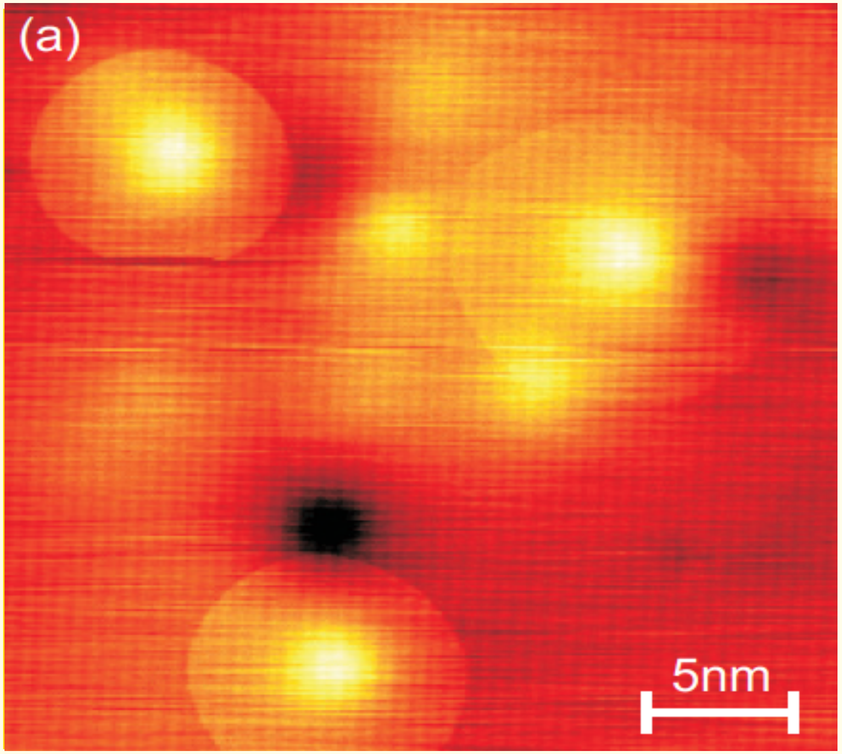
Si donors at different depths below the 110 cleavage surface



Low Temperature Imaging

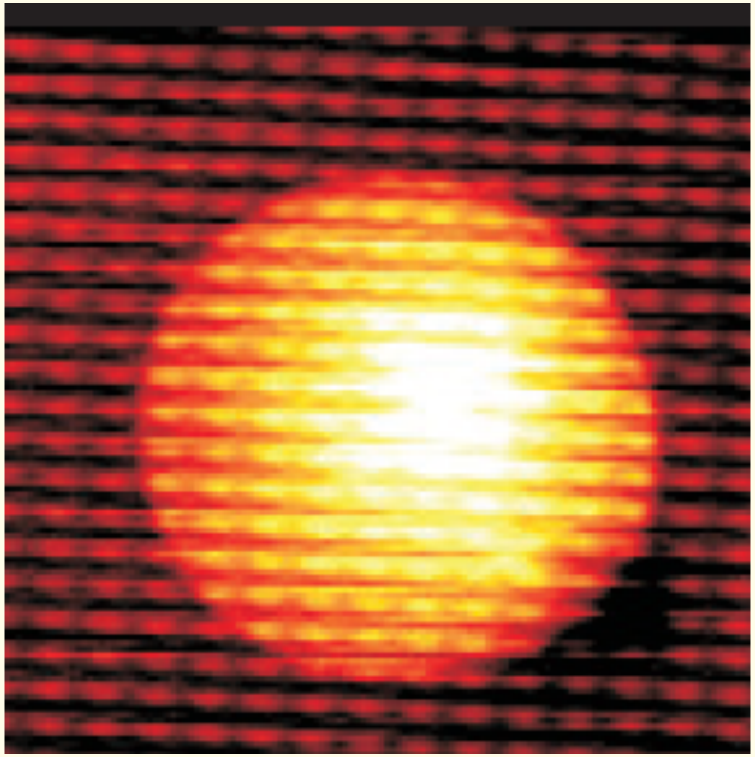
Si Doped GaAs measured at 5 K

50 nm * 50 nm



Si donors at different depths below the 110 cleavage surface

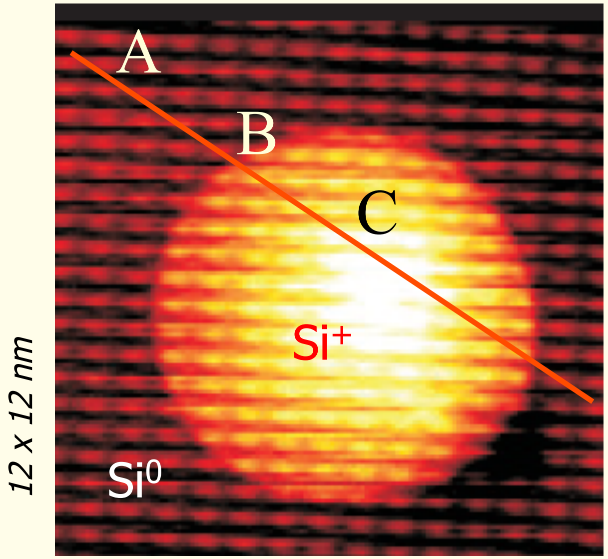
8 nm * 8 nm

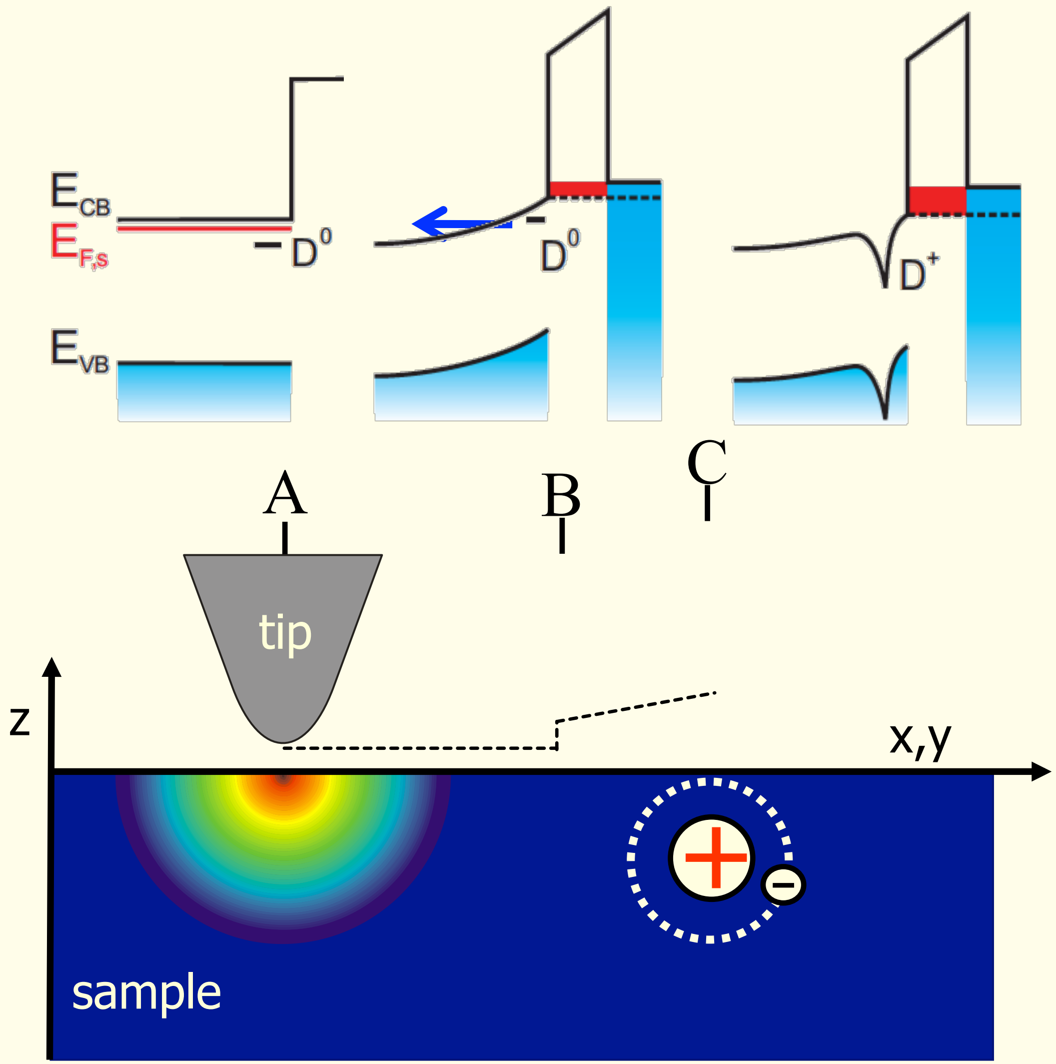


Single Si donor in GaAs

Ionization process

topography:

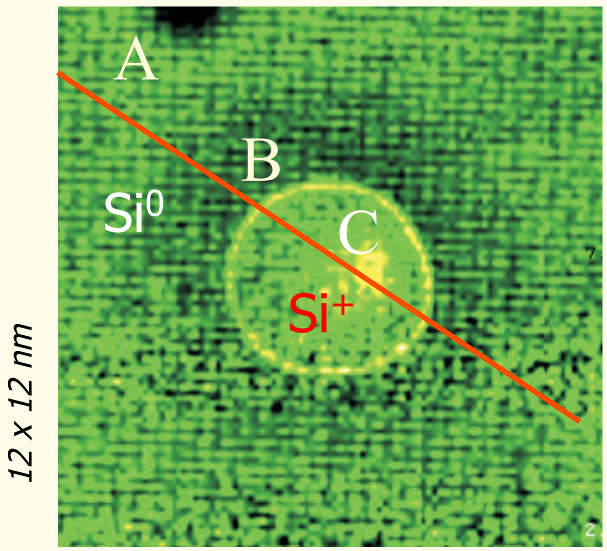




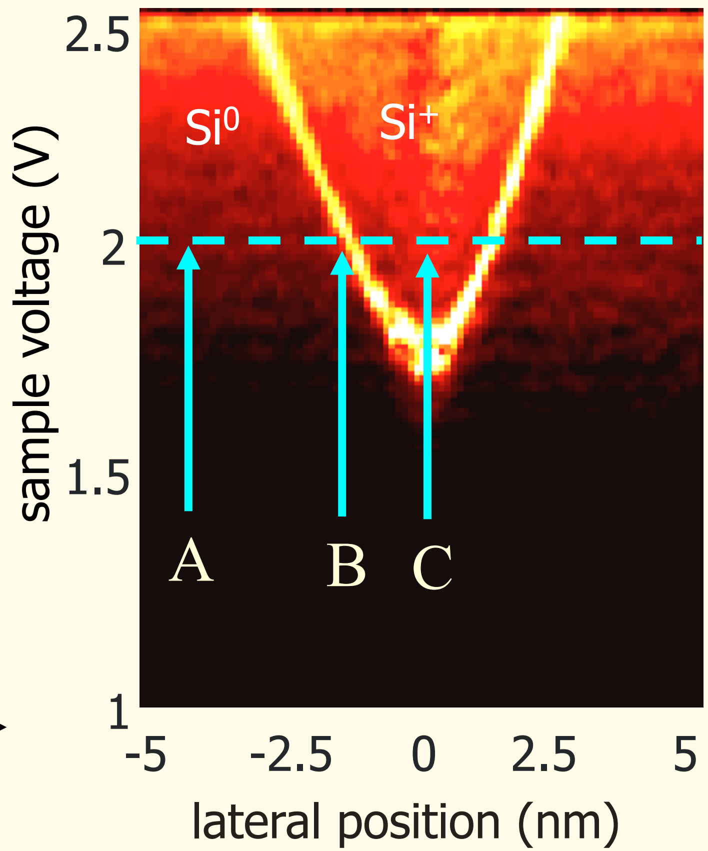
*K. Teichman et al, PRL **101**, 076103 (2008)*

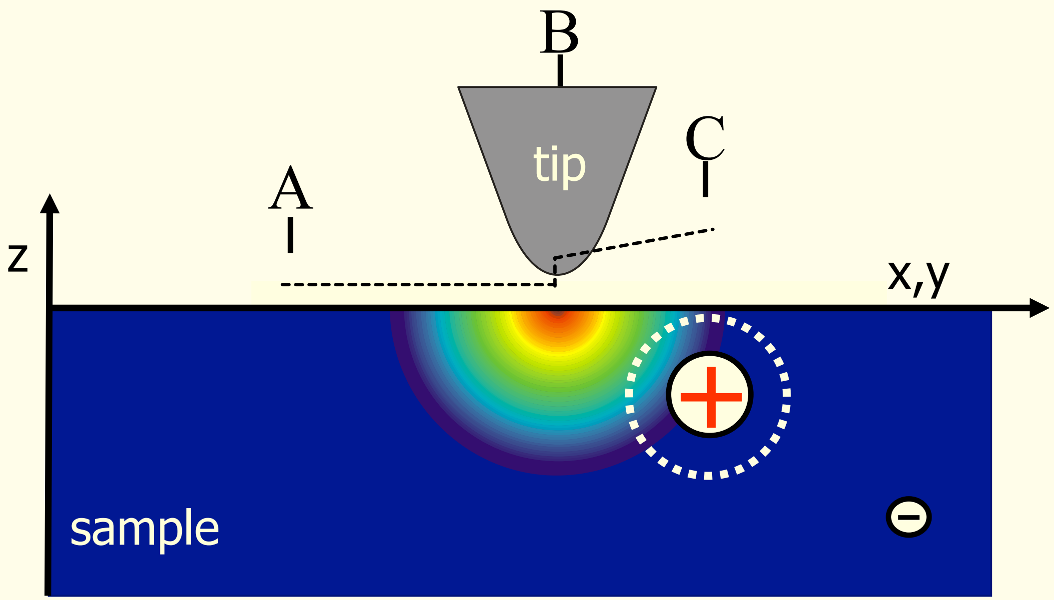
Ionization process

dI/dV topography:



differential conductivity:

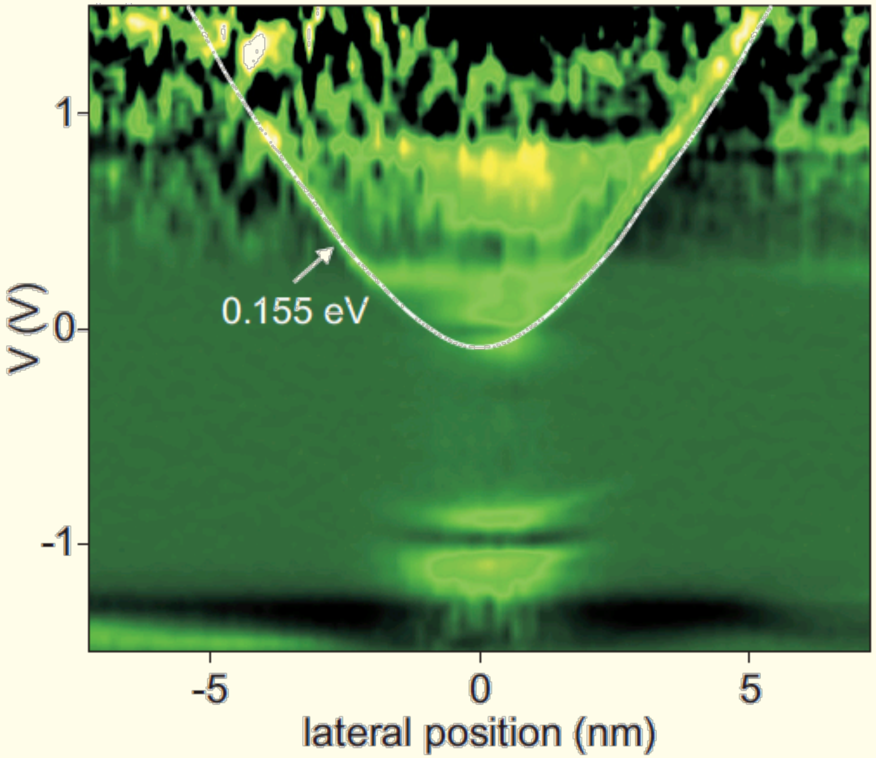


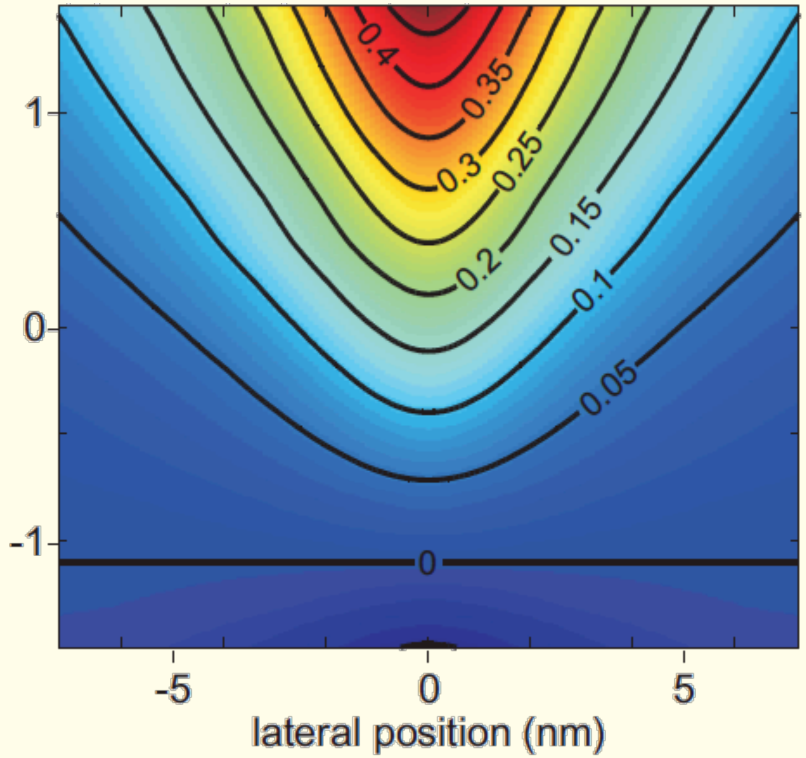


*K. Teichman et al, PRL **101**, 076103 (2008)*

Voltage Dependence

R. M. Feenstra, J.Vac. Sci. Technol B ***21****, 2080 (2003)*

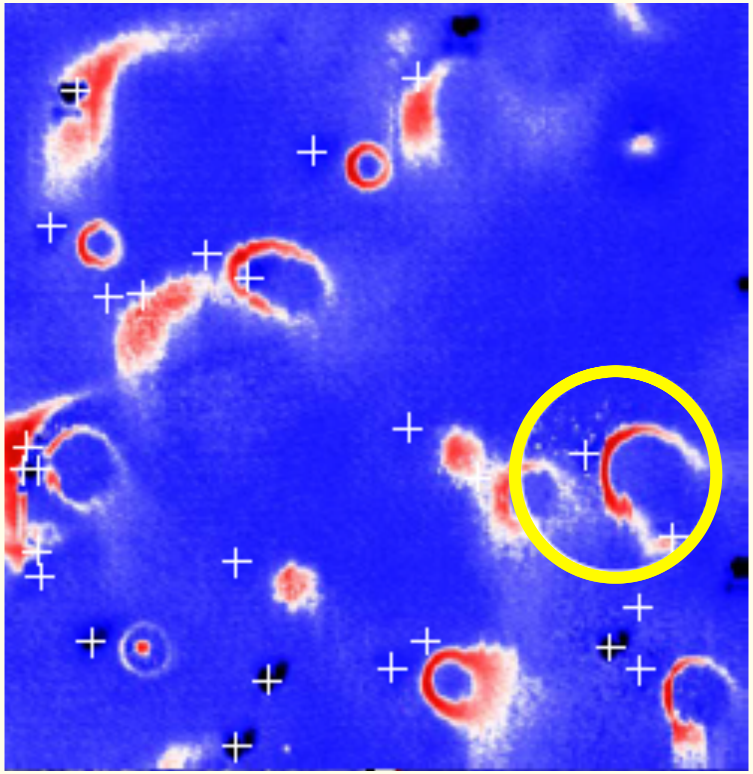




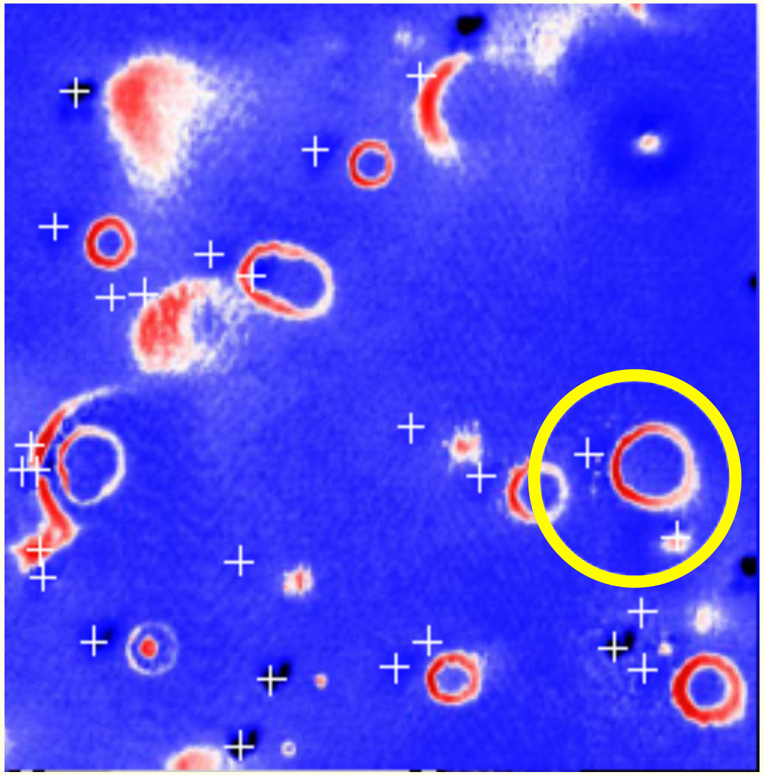
flat band voltage and tip radius are the main fitting parameters

Ionization rings for Mn in InAs

dI/dV map at 1.05 V



dI/dV map at 1.10 V



F. Marczinowski et al, PRB ***77****, 115318 (2008)*

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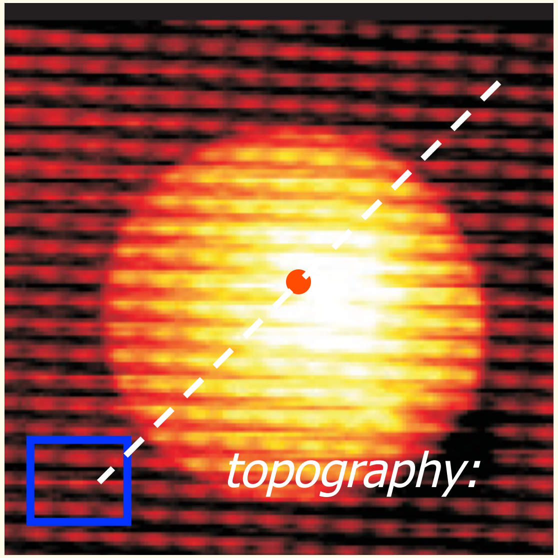
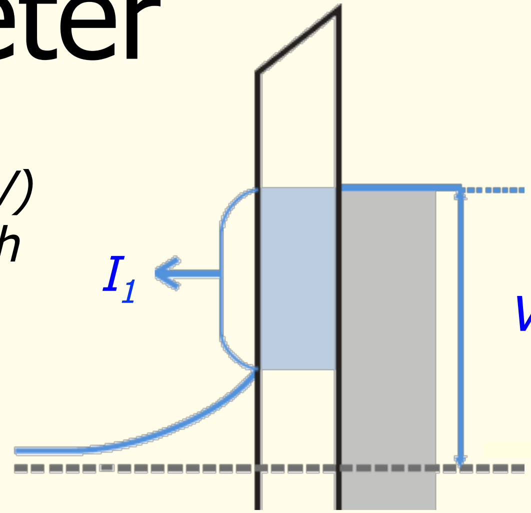
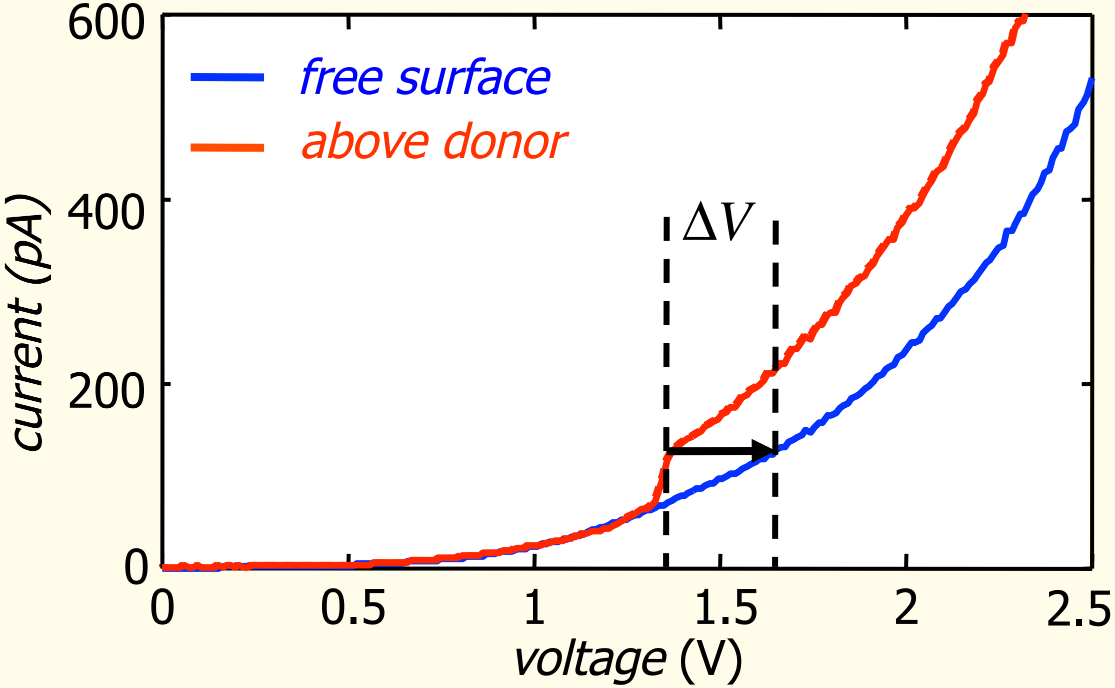
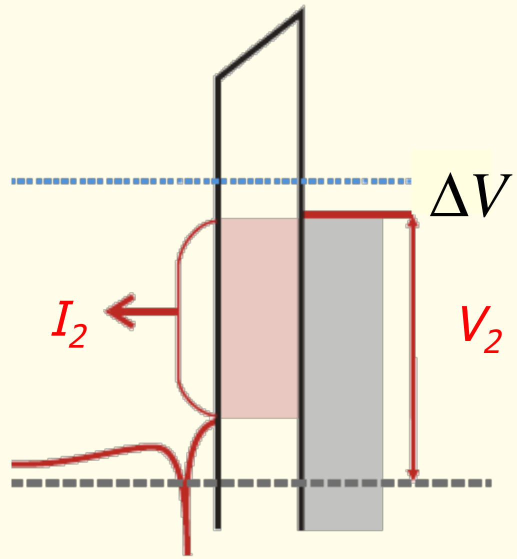


Potentiometer

The shift $\Delta V(r)$ in the I(V) spectra corresponds with the local potential

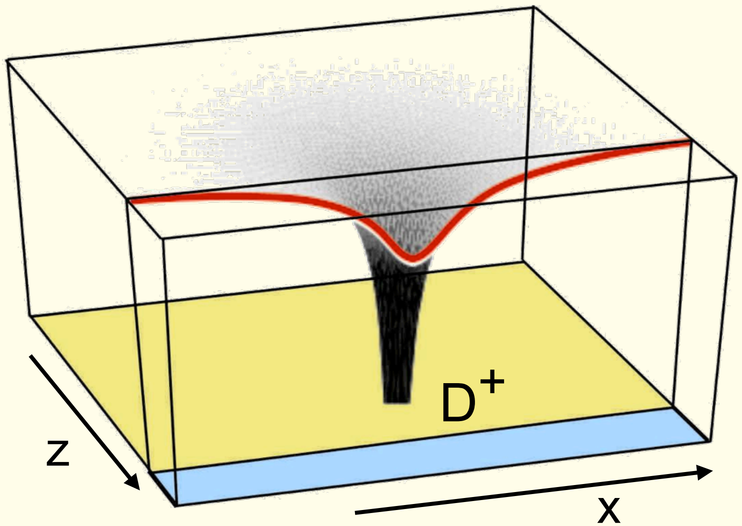


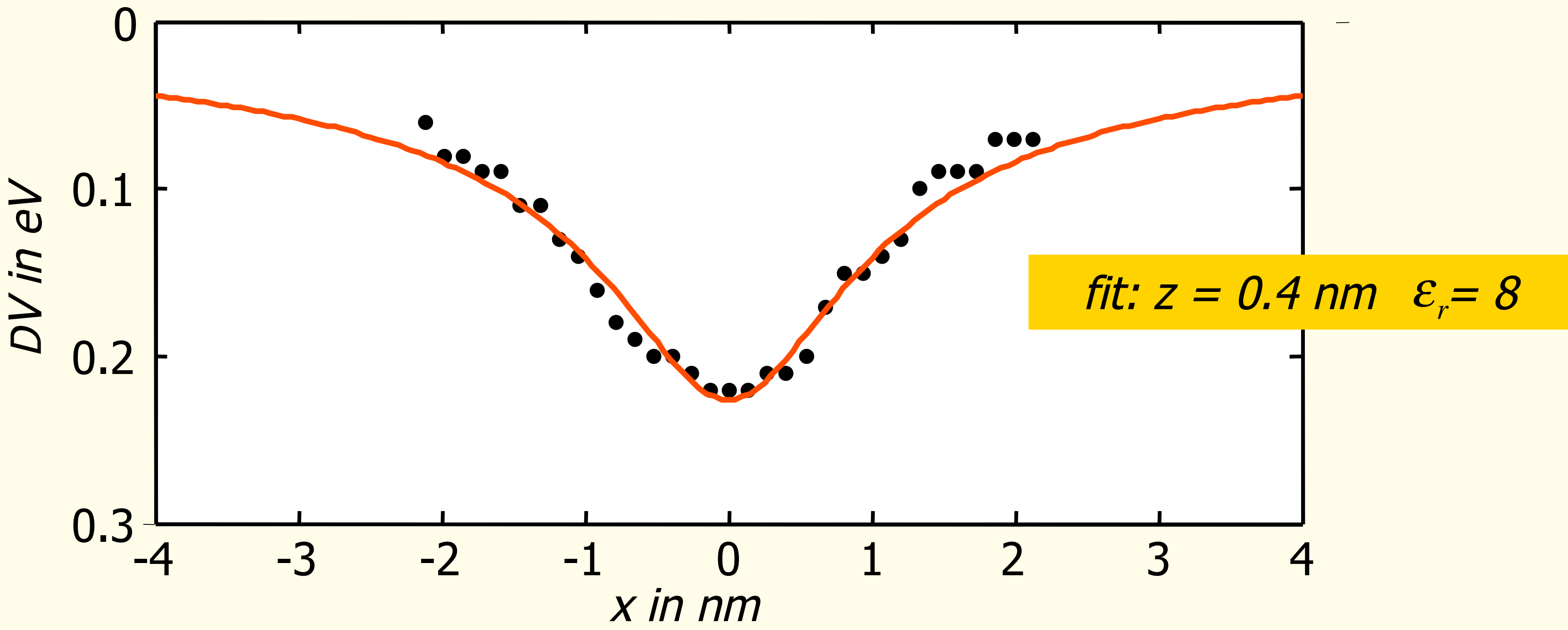




Coulomb Potential of a near surface Donor

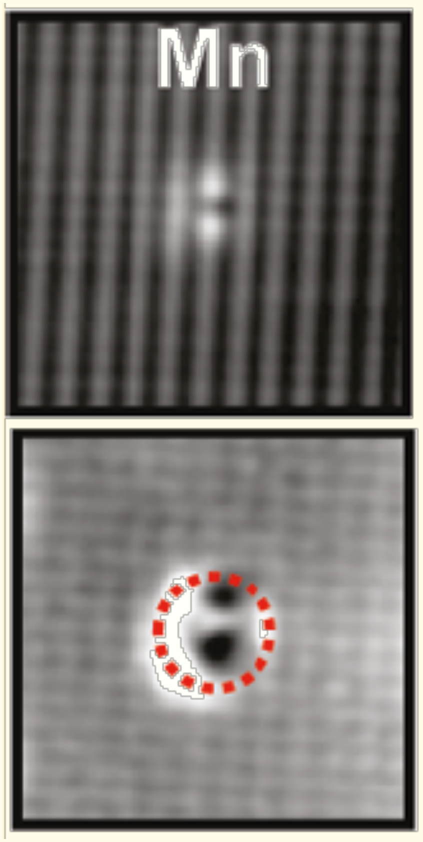
$$V = \frac{1}{4\pi\varepsilon_0\varepsilon_r}\frac{1}{(x^2+z^2)^{1/2}}$$



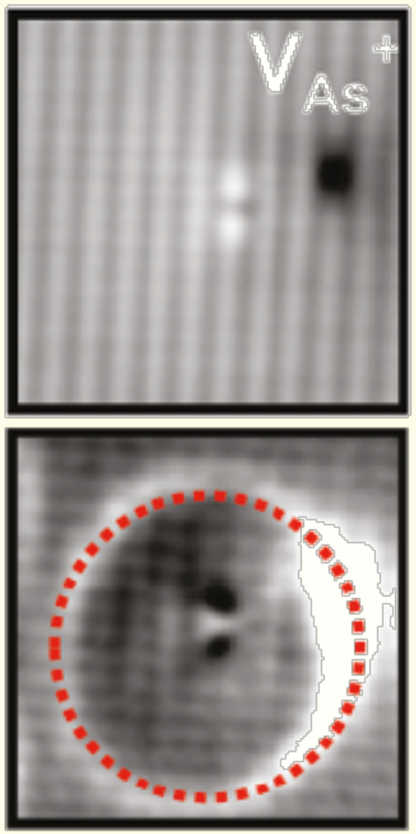


*K. Teichman et al, PRL **101**, 076103 (2008)*

Coulomb Profiling with an As-vacancy



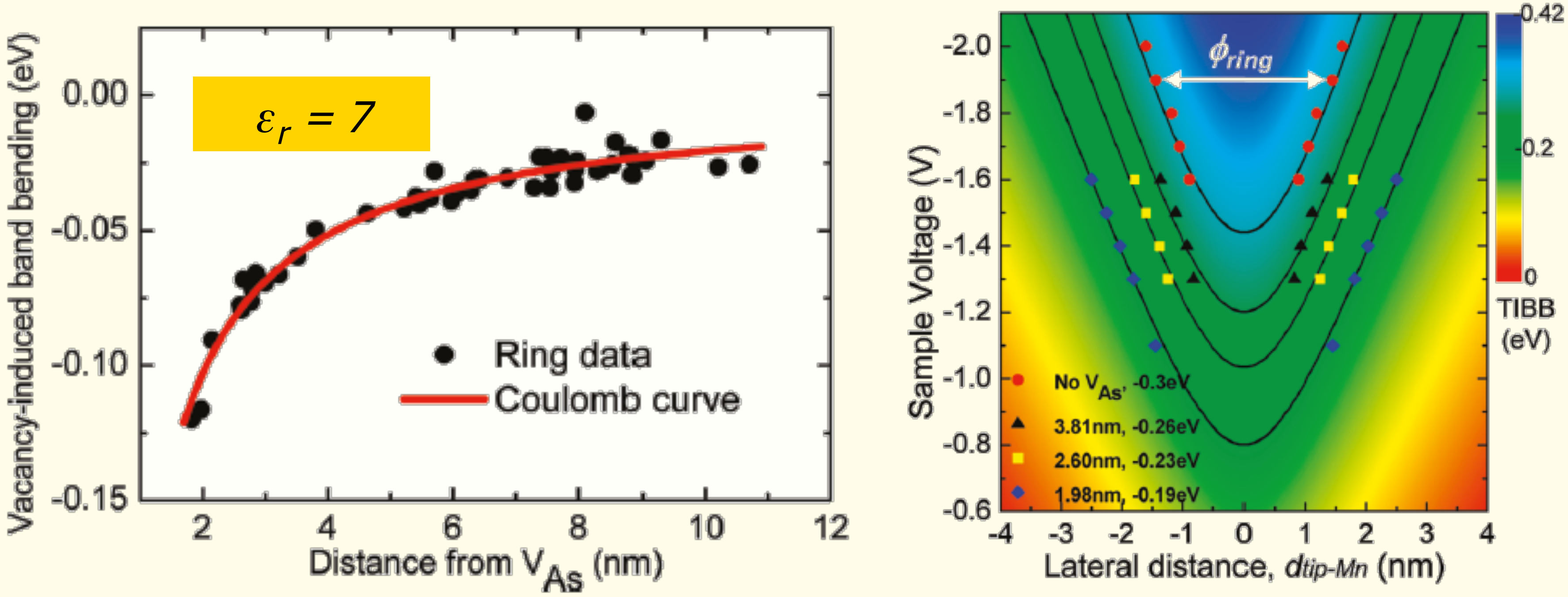
STM induced creation of As-vacancy near Mn in GaAs



D. Lee and J. Gupta, NanoLetters ***11****, 2004 (2011)*

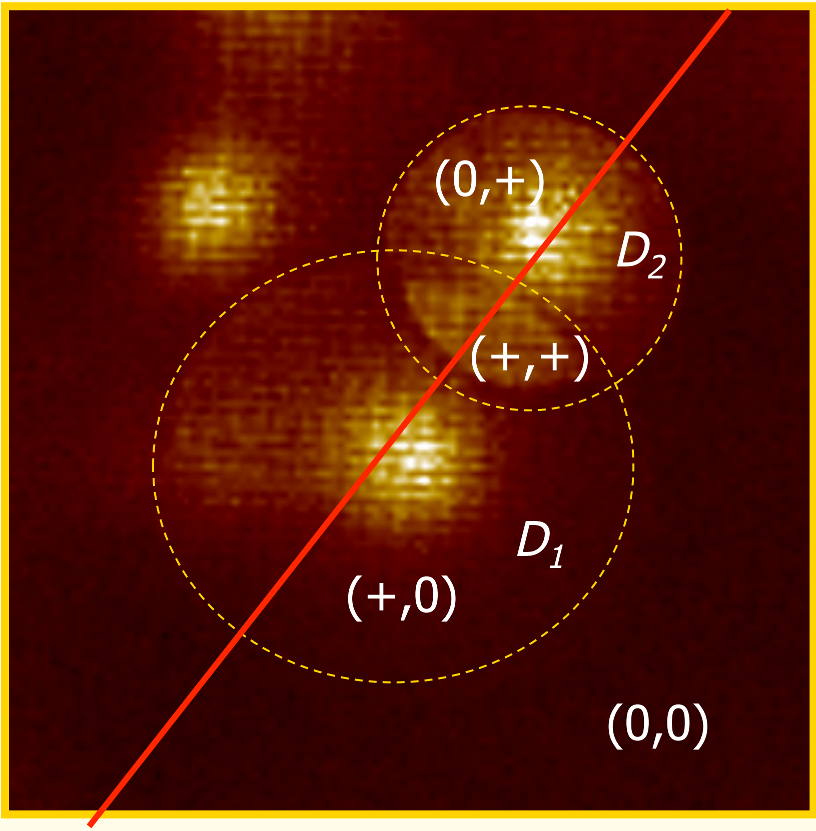
Coulomb Profiling with an As-vacancy

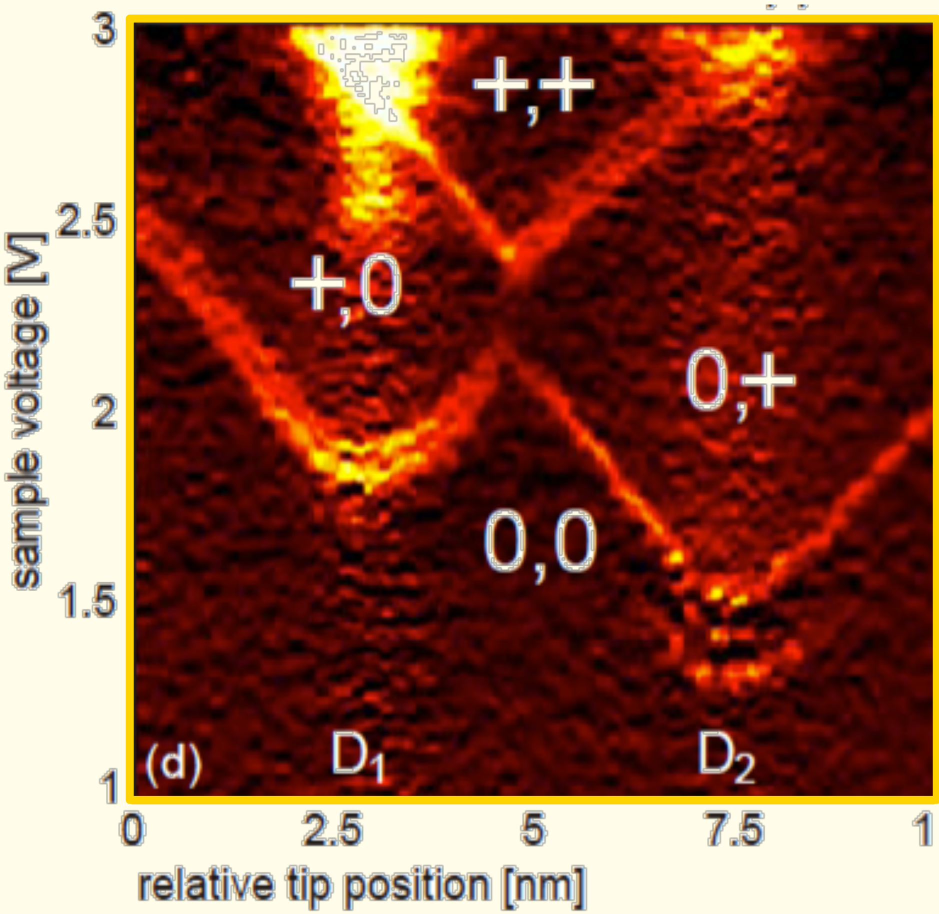
As-vacancy at surface is a singly charged donor



*D. Lee and J. Gupta, NanoLetters **11**, 2004 (2011)*

Coulomb Interaction

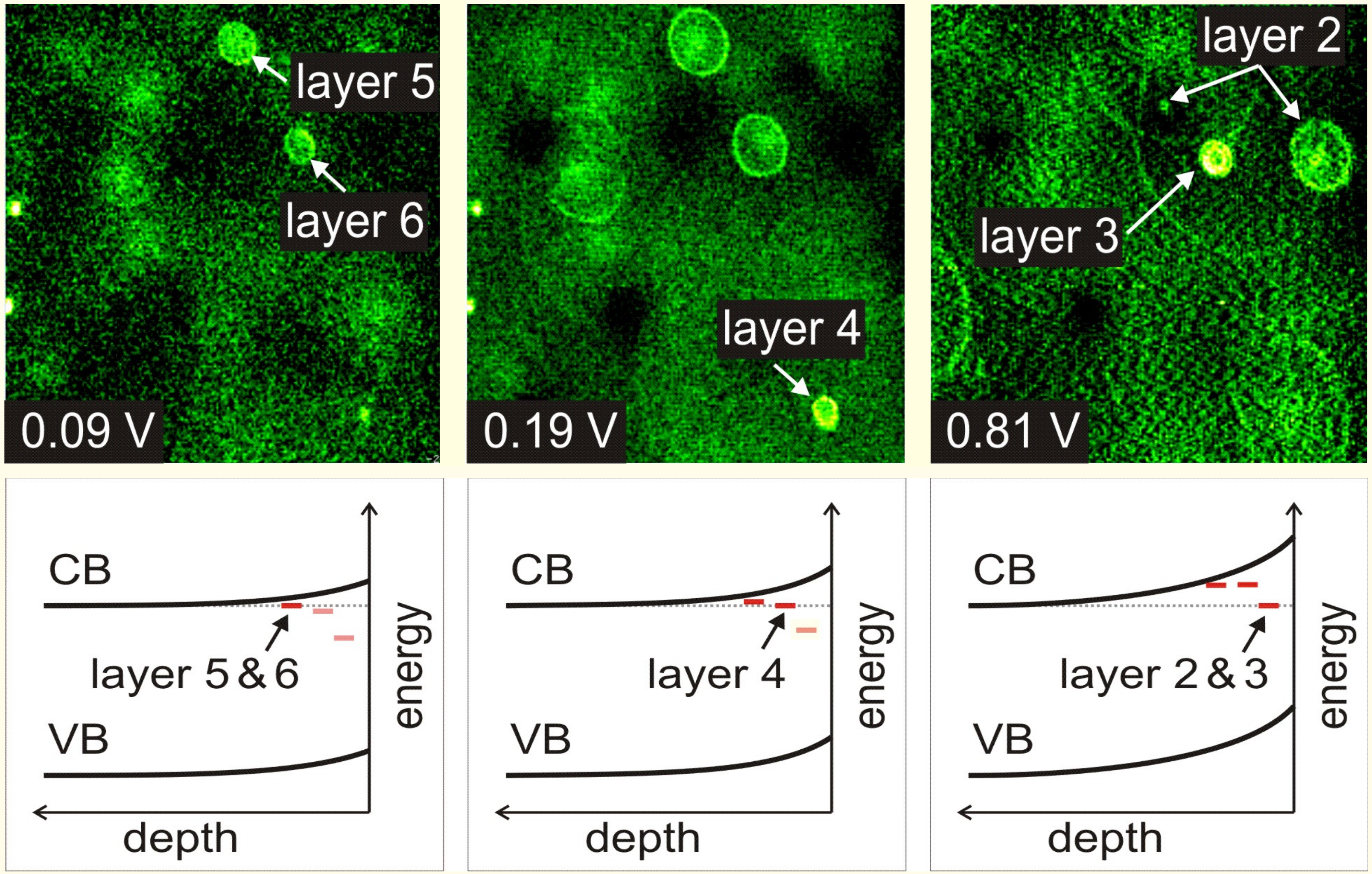




(D_1,D_2) = charge state donor pair

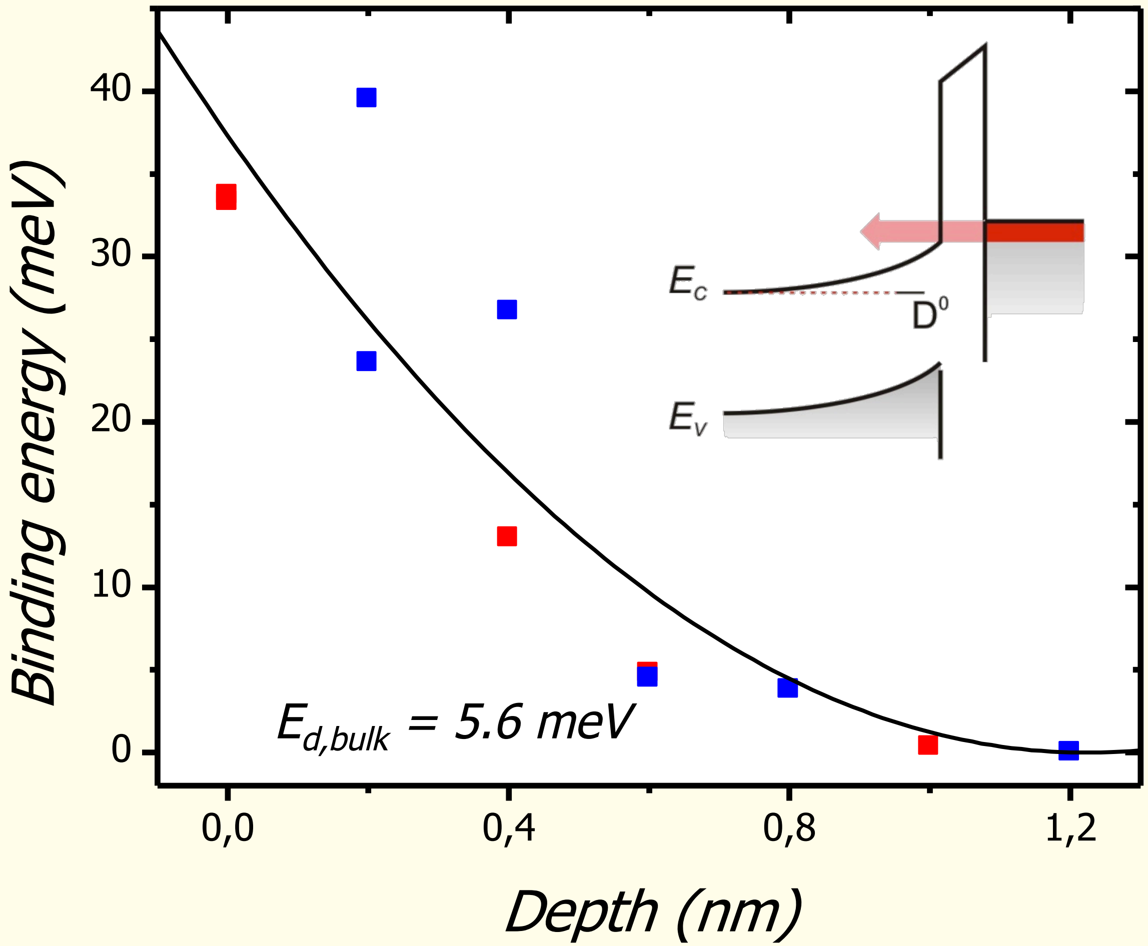
K. Teichman et al, submitted for publication

Depth Dependent Binding Energy



*A.P. Wijnheijmer et al PRL **102**, 166101 (2009)*

Depth Dependent Binding Energy



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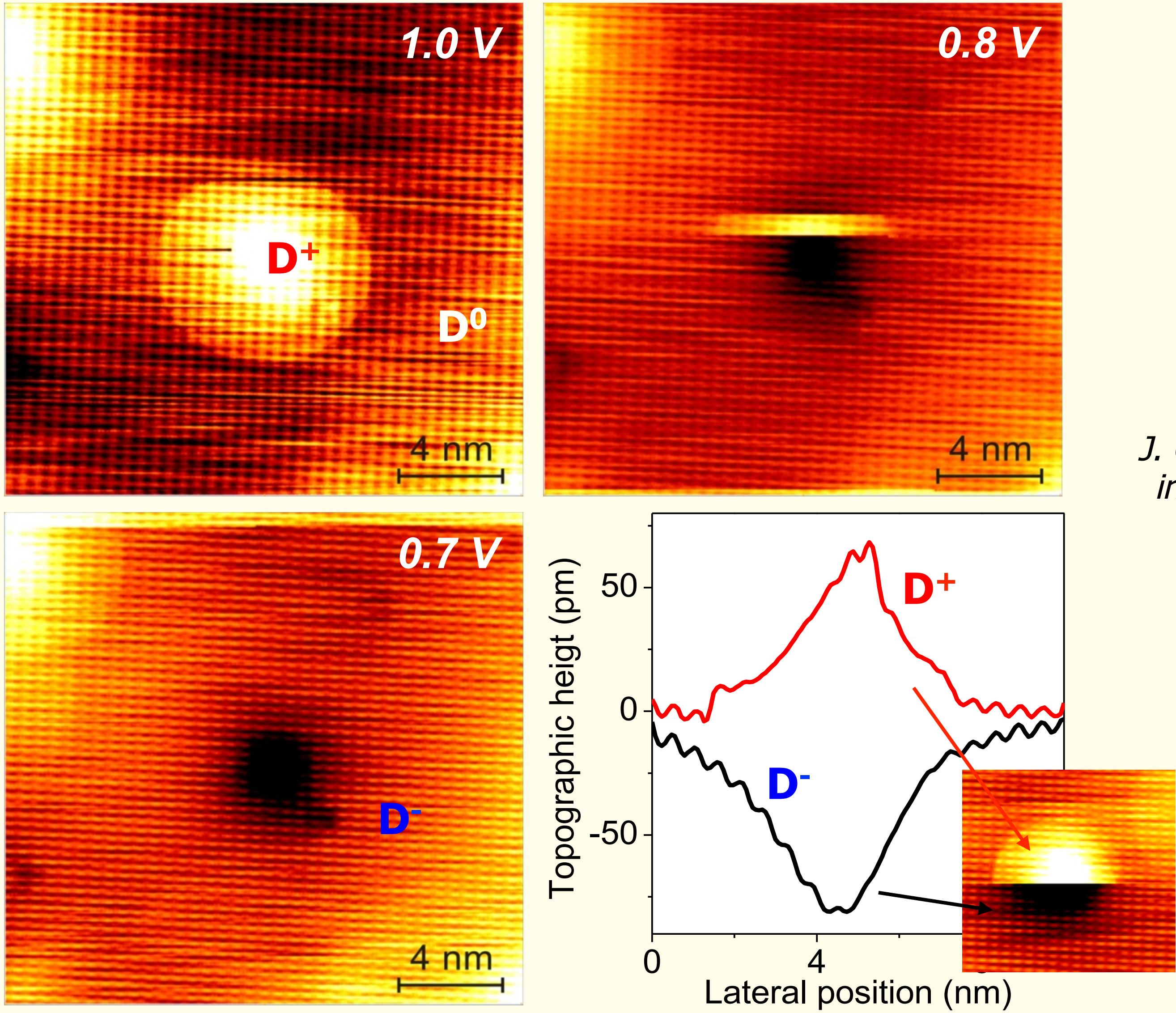
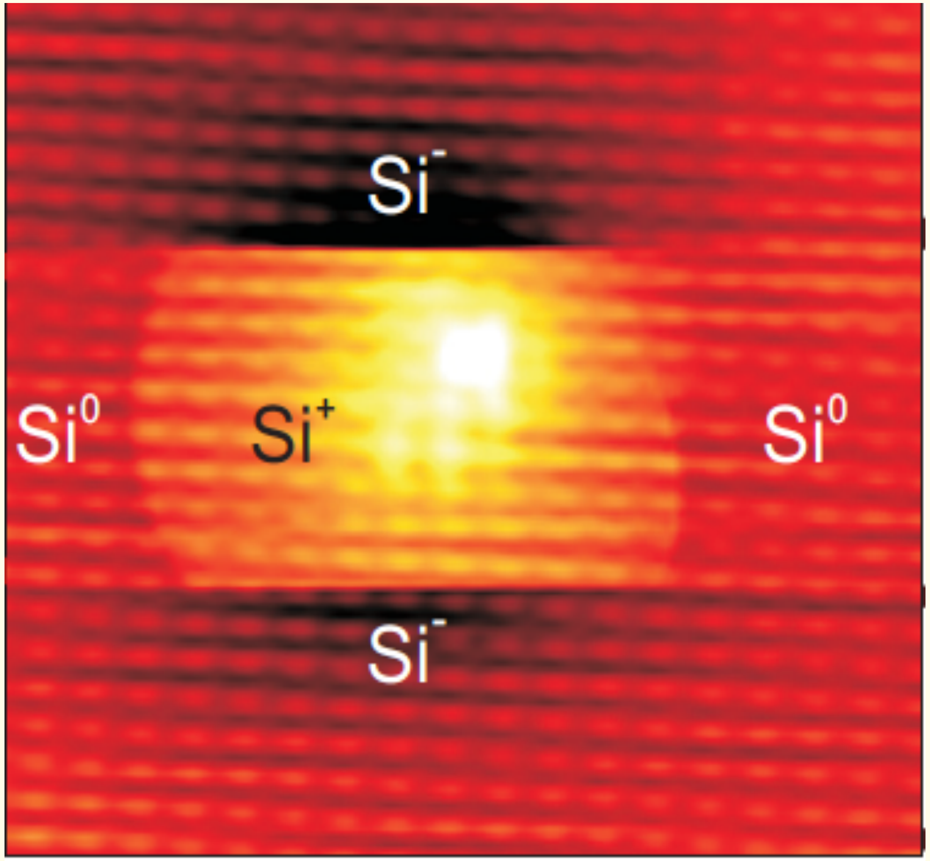
Switching of Si in the Surface Layer



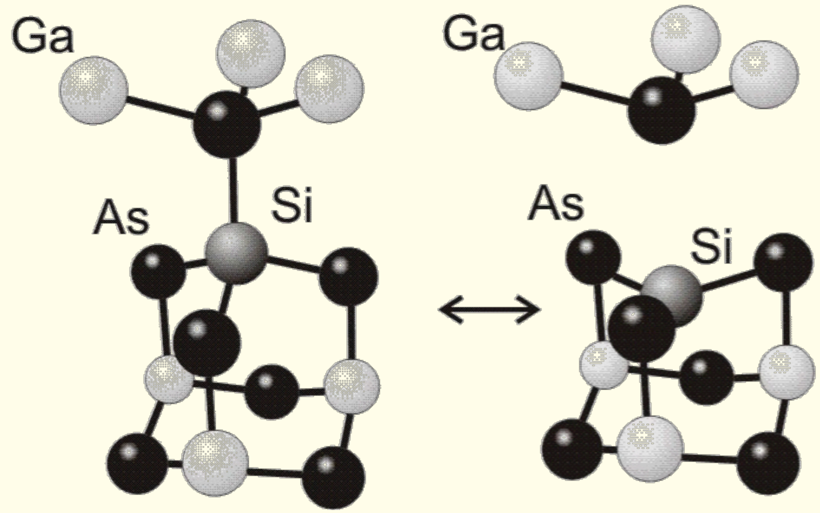
J. Garleff et al,
in press PRB

Bond Reconfiguration



Only observed for Si donors in the topmost layer

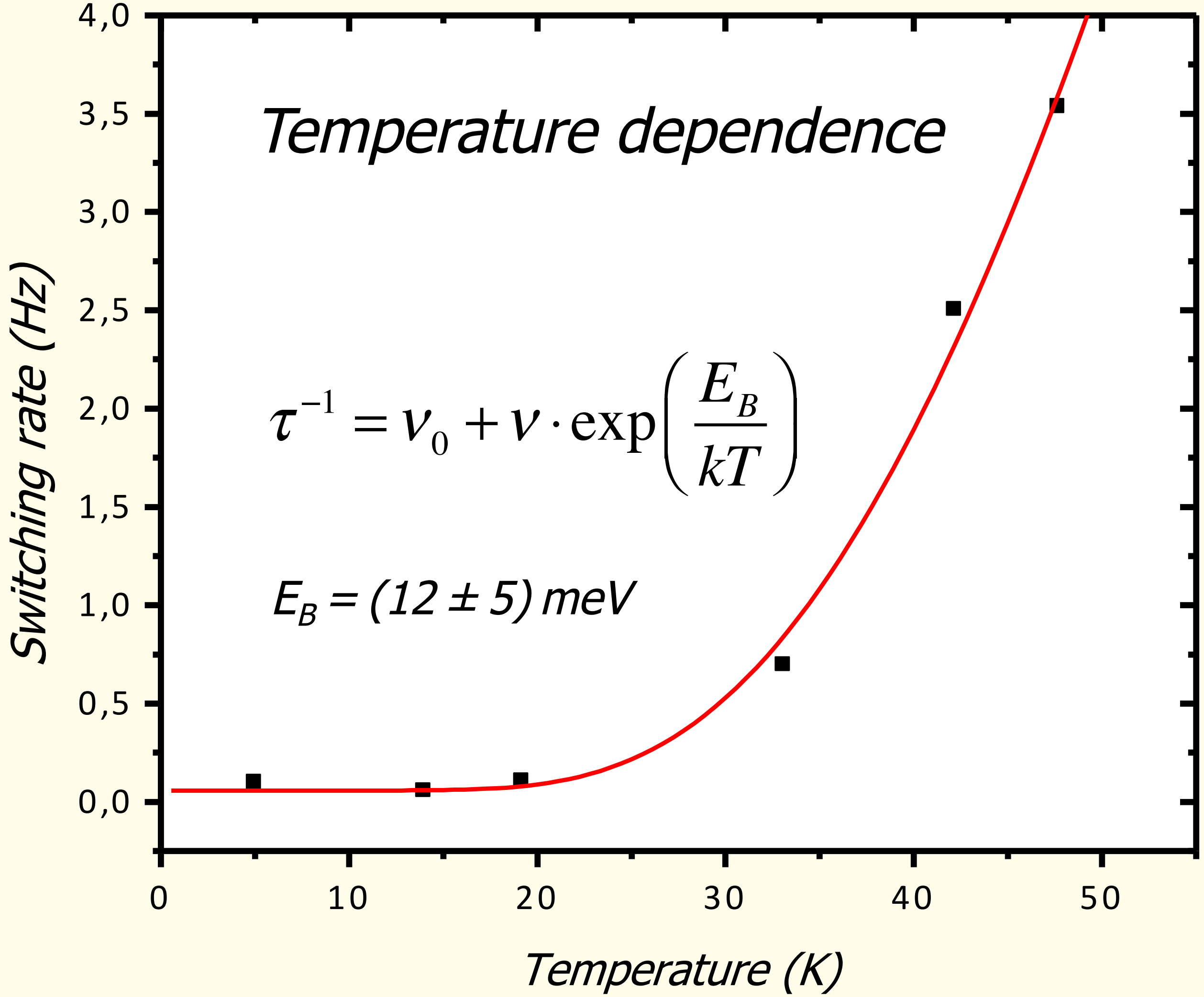
Substitutional position | *Interstitial position*

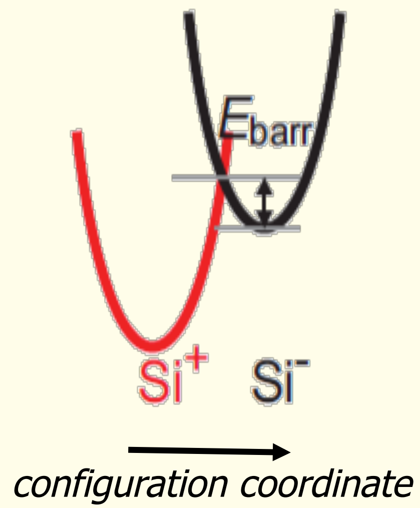


$d^+ + e$ | " DX^- "

P. Mooney, Semi. Sci & Technol. ***6****, B1 (1991)*

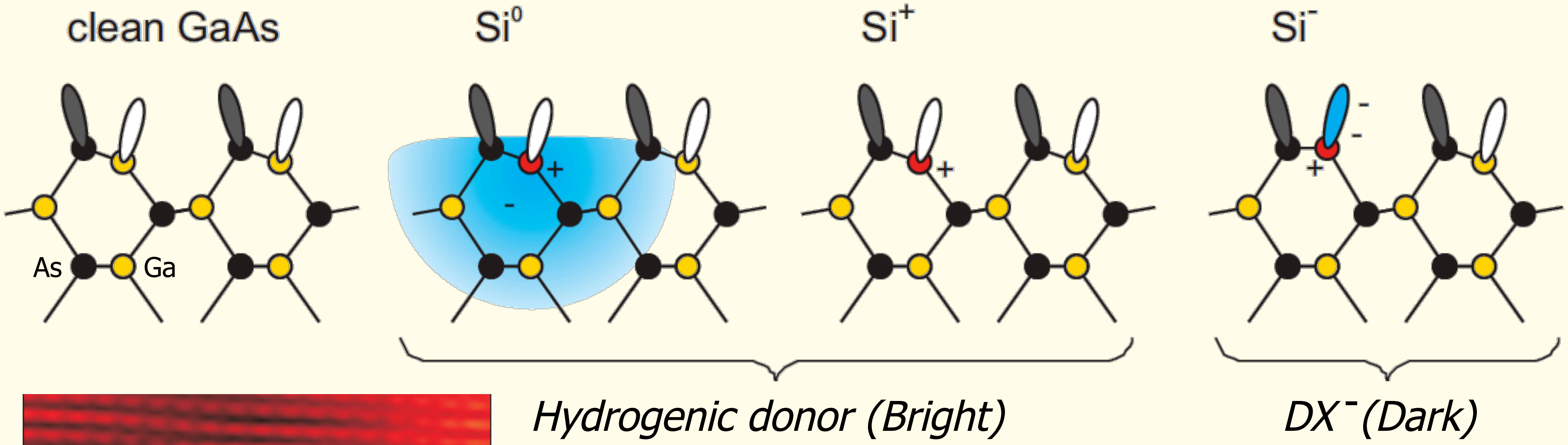
Si^+ / Si^- - Switching Rate

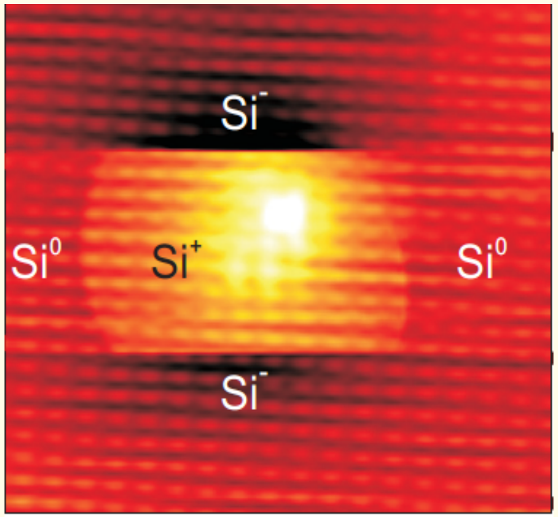




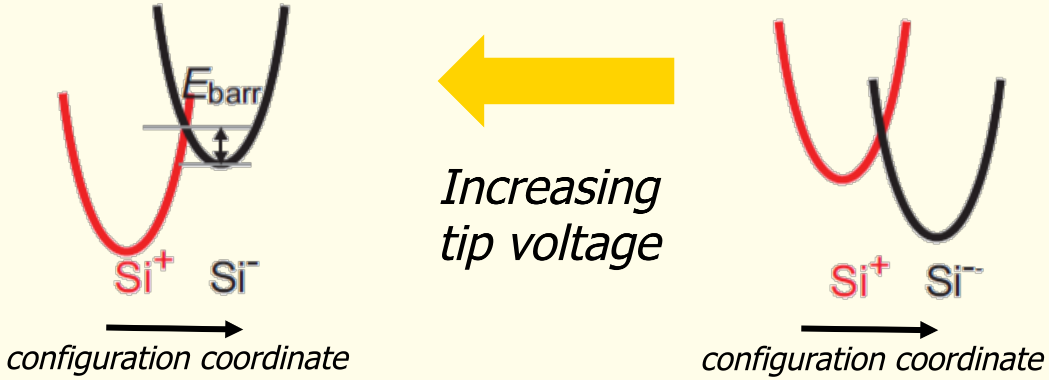
J. Garleff et al, in press PRB

Impurity Model





J. Garleff et al, in press PRB



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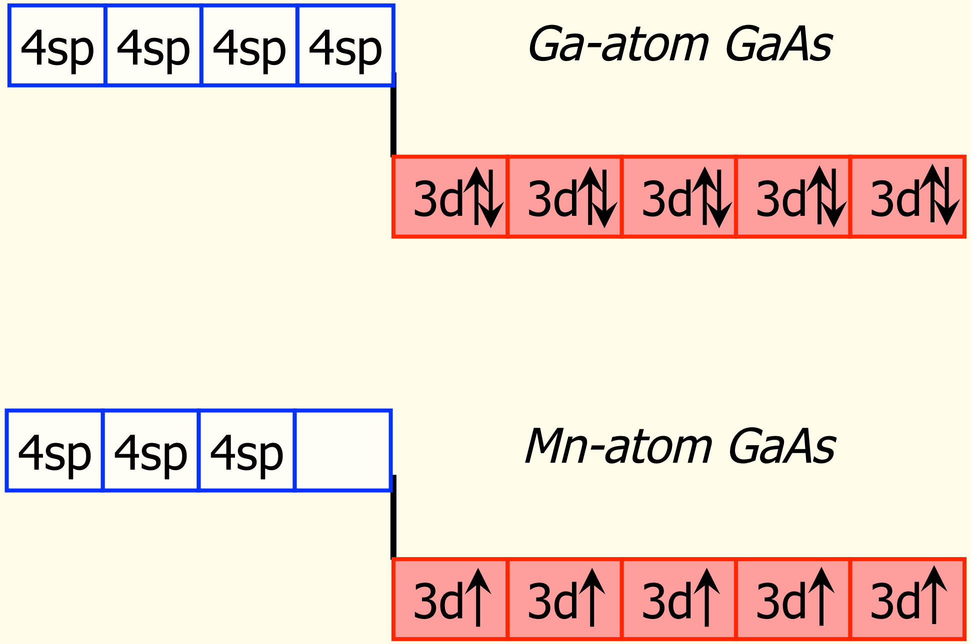
Electronic Structure

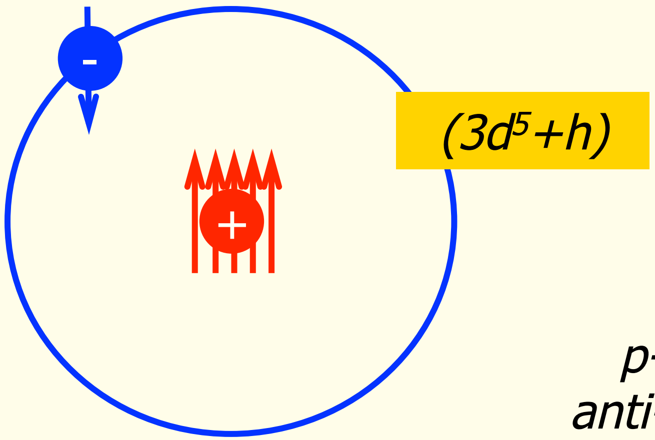
magnetic doping: a part of the atoms in the crystal is replaced by magnetic transition metal impurities

Ga-atom GaAs



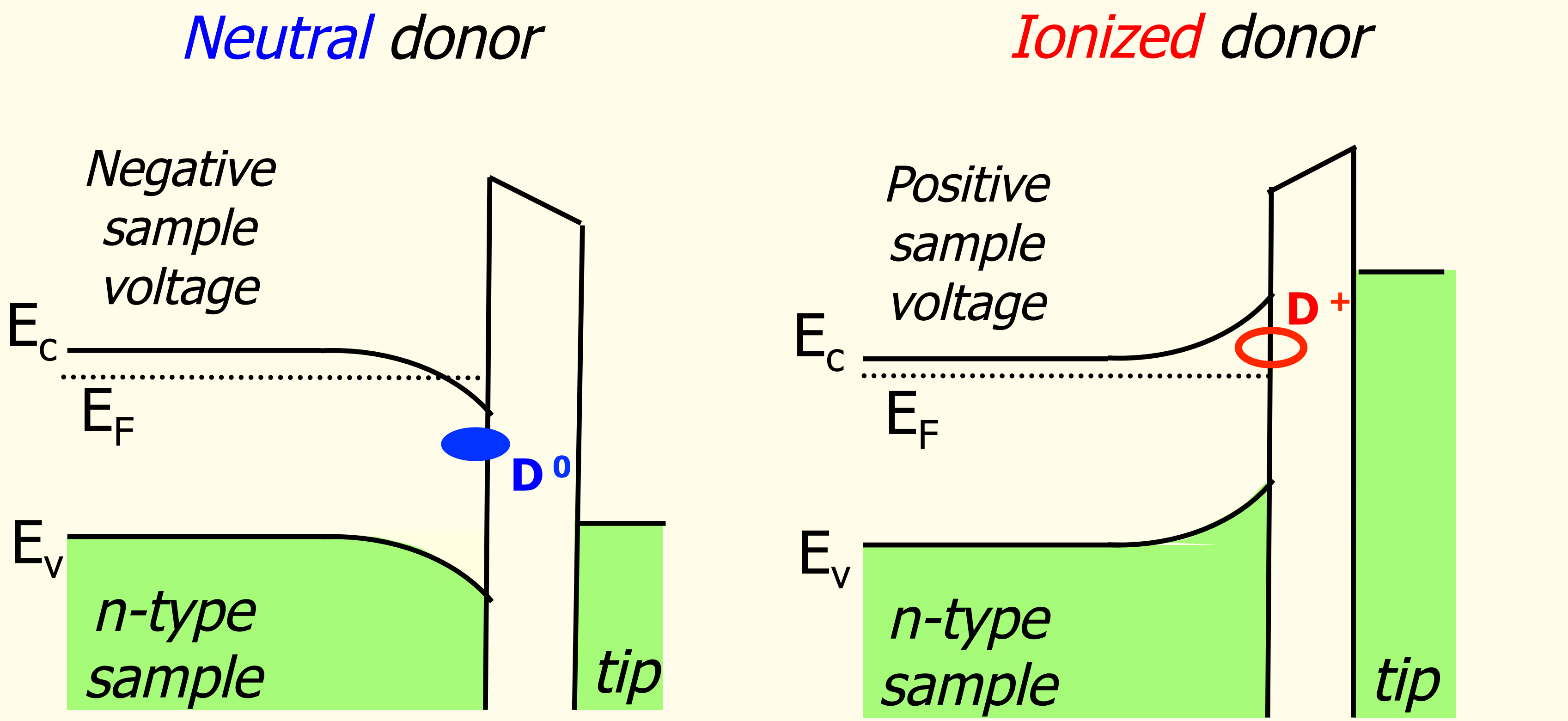
Mn-atom GaAs

Mn on Ga-site in GaAs

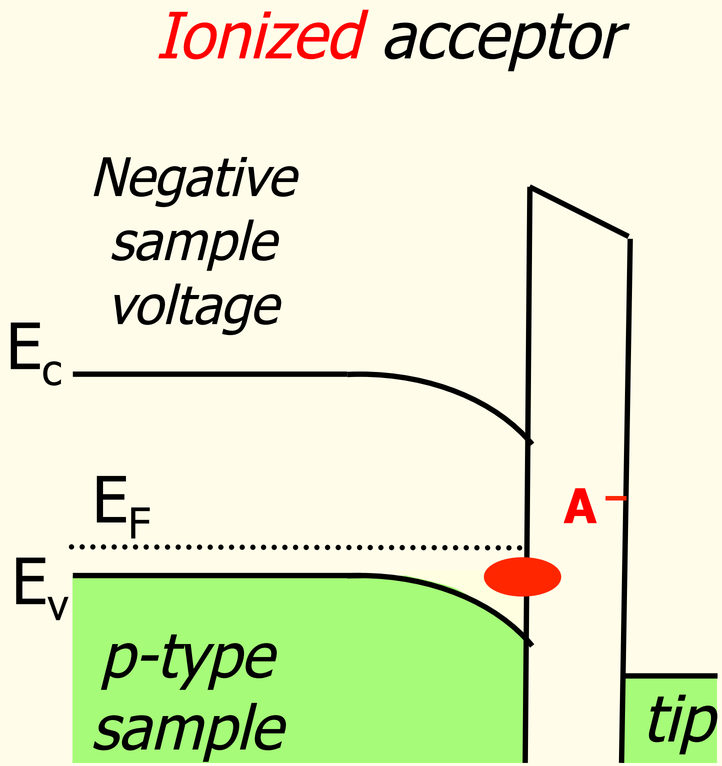


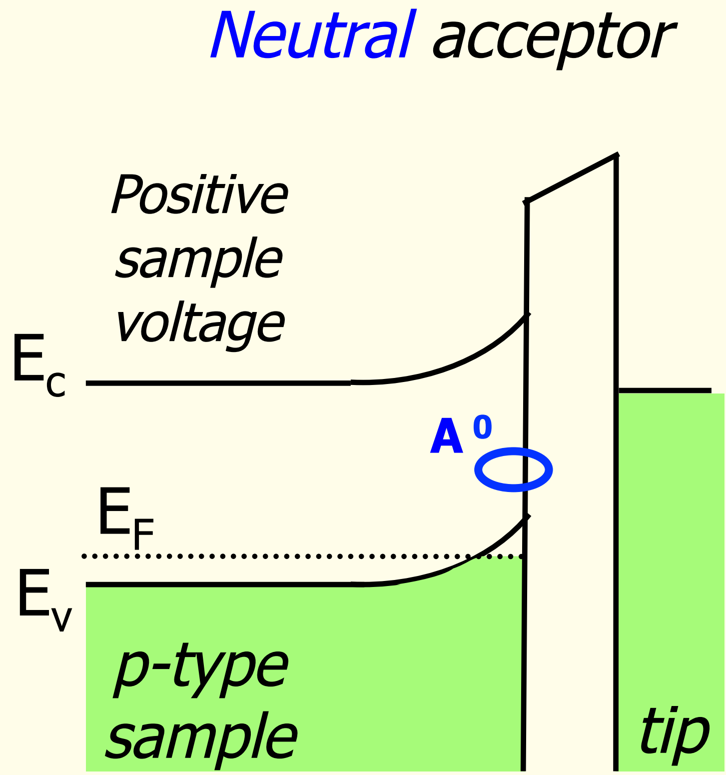
p-d interaction results in anti-ferromagnetic alignment

Manipulation of the Charge State by an STM tip



Manipulation of the Charge State by STM tip

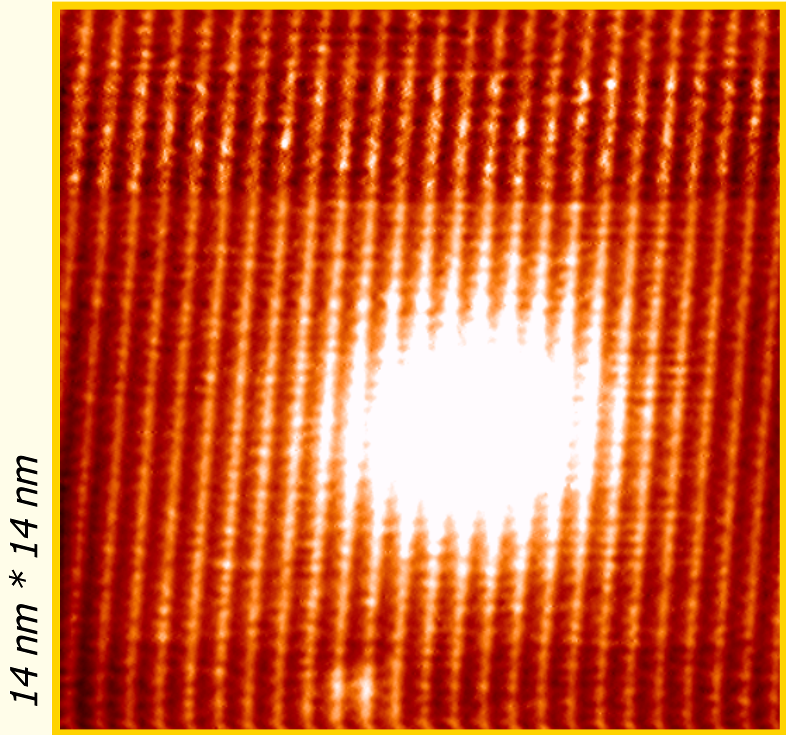




A^- and A^o Charge States of Mn

Ionized *Mn* A^-

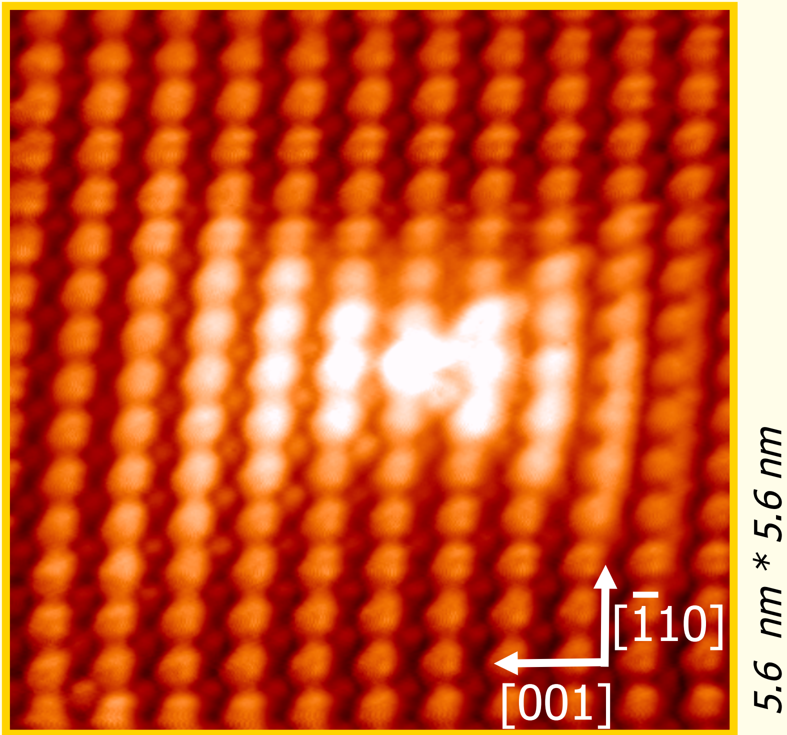
(V=-0.9 V)



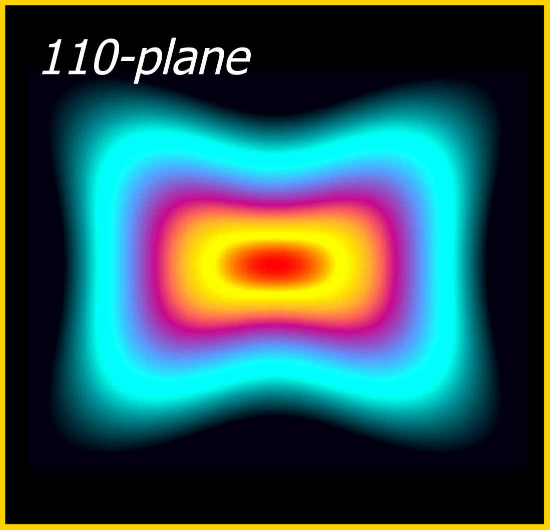
Contrast is due to Coulomb field

Neutral *Mn* A^o *(ion + hole)*

(V=+0.7 V)



Tunneling to the bound hole
(Mn in ~ 3rd sublayer)



Luttinger Hamiltonian

$$H_{Lut}(k_x,k_y,k_z)\psi_i + V(r)\psi_i = \varepsilon_i \psi_i$$

<u>Luttinger Hamiltonian</u>

$$H_{Lut}(k_x,k_y,k_z) = \frac{\hbar^2}{2m_o}\begin{bmatrix} H_{hh} & c & -b & 0 \\ c^+ & H_{lh} & 0 & b \\ -b^+ & 0 & H_{lh} & c \\ 0 & b^+ & c^+ & H_{hh} \end{bmatrix}$$

$$\psi_i = \begin{pmatrix} \phi_1 \cdot |3/2,+3/2\rangle \\ \phi_2 \cdot |3/2,+1/2\rangle \\ \phi_3 \cdot |3/2,-1/2\rangle \\ \phi_4 \cdot |3/2,-3/2\rangle \end{pmatrix}$$

4-vector representation based on spin-projection

$$H_{hh} = \left(k_x^2 + k_y^2\right)\left(\gamma_1 + \gamma_2\right) + k_z^2\left(\gamma_1 - 2\gamma_2\right)$$

$$H_{lh} = \left(k_x^2 + k_y^2\right)\left(\gamma_1 - \gamma_2\right) + k_z^2\left(\gamma_1 + 2\gamma_2\right)$$

$$b = 2\sqrt{3}\gamma_3(k_x - ik_y)k_z$$

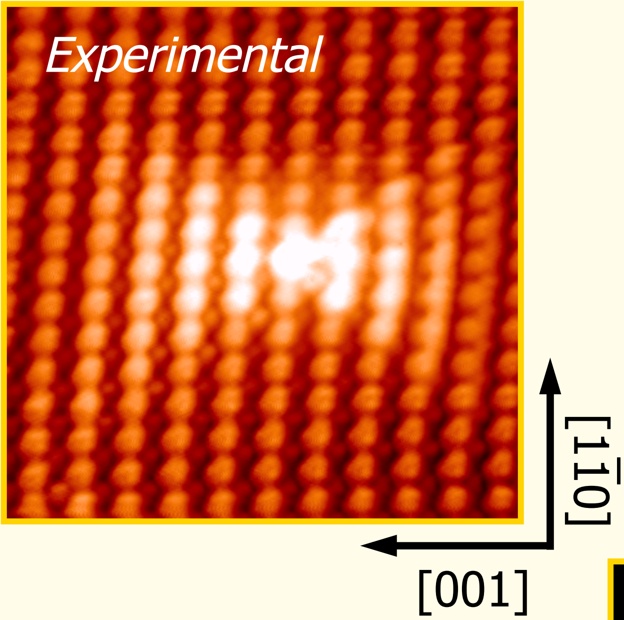
$$c = -\sqrt{3}\left[\gamma_2\left(k_x^2 - k_y^2\right) - 2i\gamma_3 k_x k_y\right]$$

γ_1, γ_2 and γ_3 Luttinger parameters

In confined systems the light and heavy hole bands are mixed

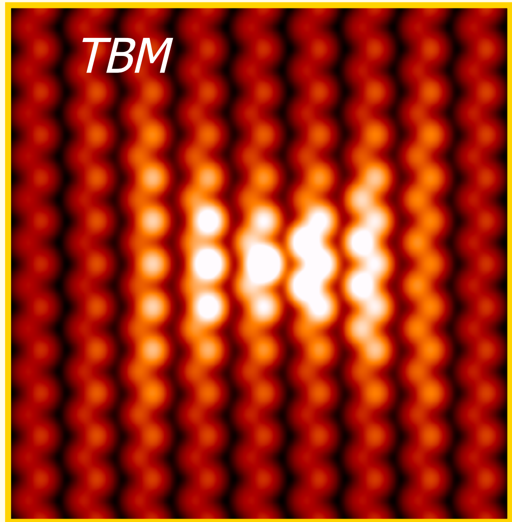
$\gamma_2 = \gamma_3$ isotropic dispersion

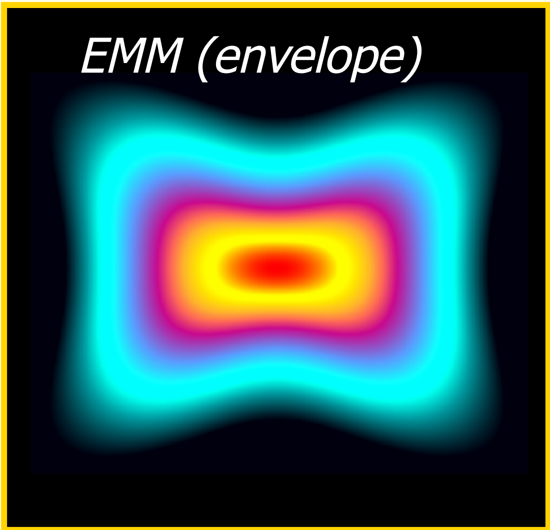
Modelling of Acceptors



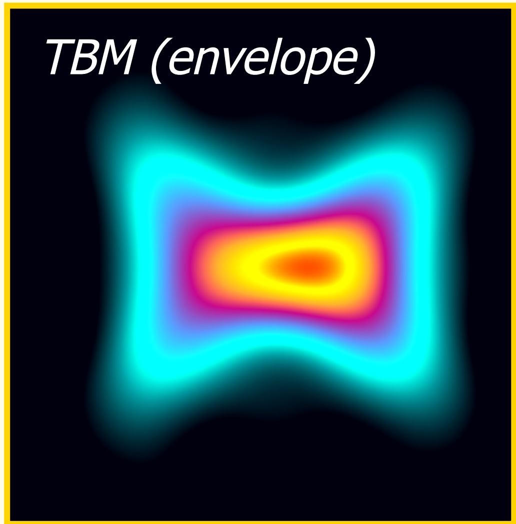
Cubic symmetry selects d-states contributing to the ground state envelope with T_2 symmetry

Yakunin et al. PRL ***92****, 216806 (2004)*

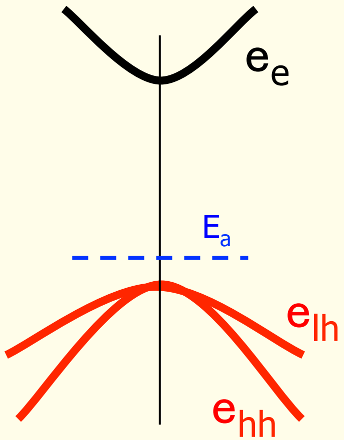




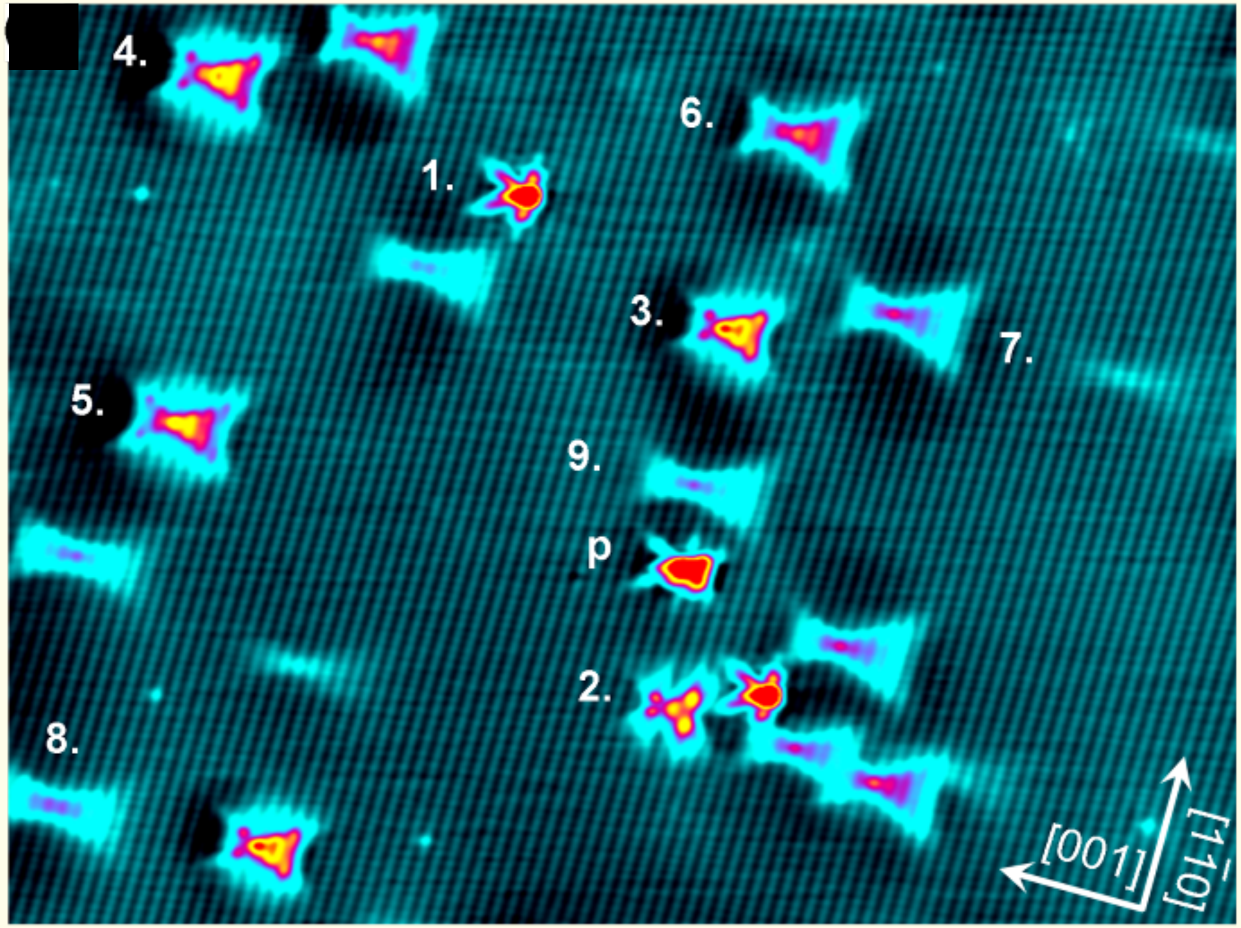
A. Monakhov, Ioffe, Russia



J.-M. Tang and M. Flatté, Iowa, US



Mn Doped GaAs



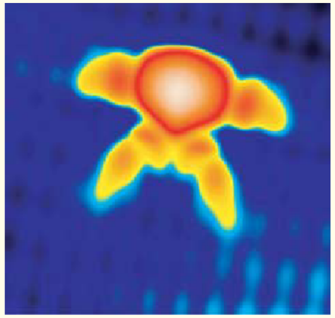
Measured at 5K

*Garleff et al PRB **78** 075313 (2008)*

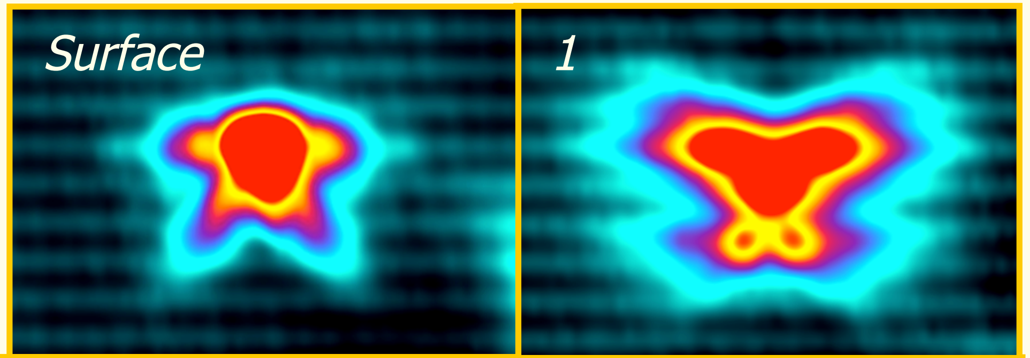
*Celebi et al PRL **104**, 086404 (2010)*

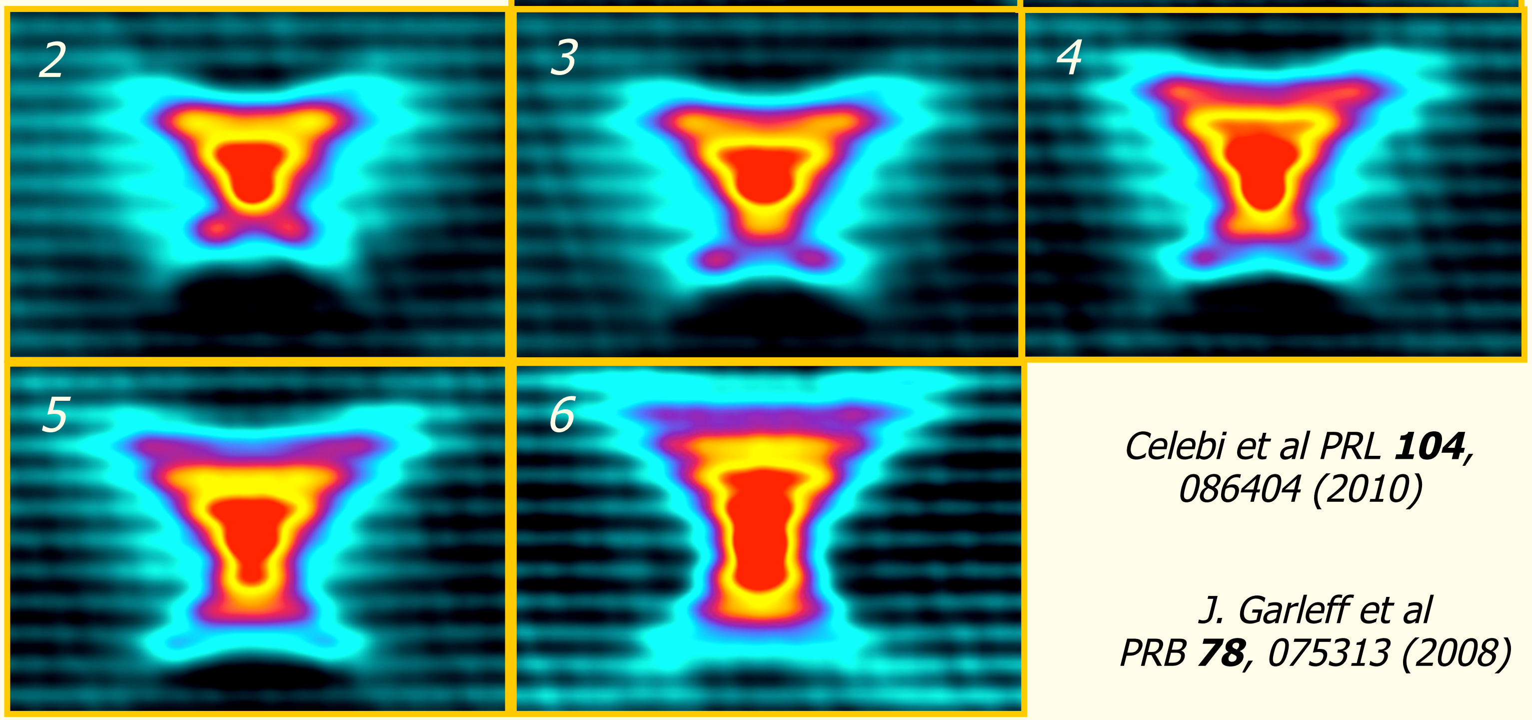
Depth dependent contrast

*Kitchen et al., Nature **442**, 436 (2006)*



Surface Mn

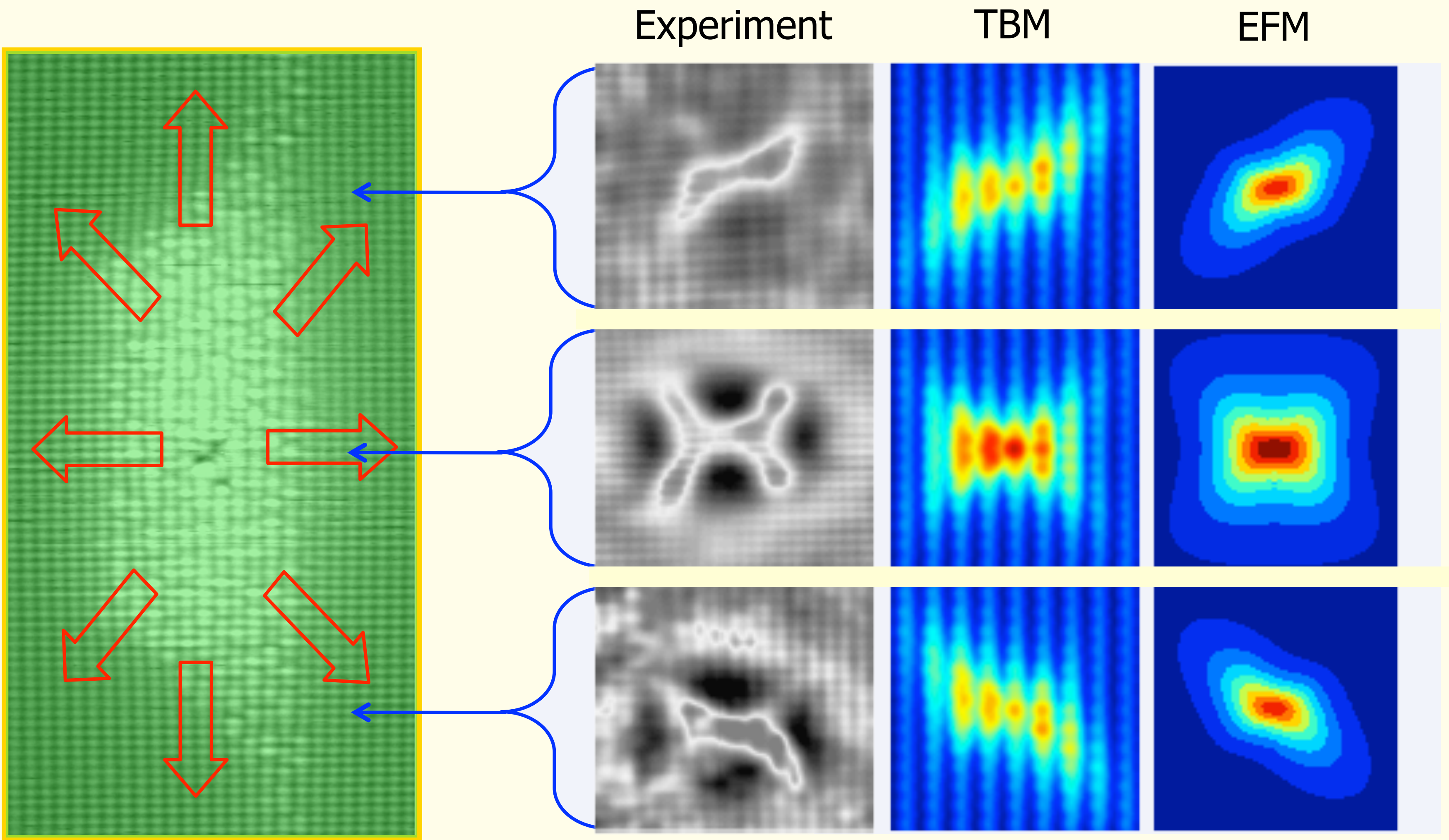




*Celebi et al PRL **104**, 086404 (2010)*

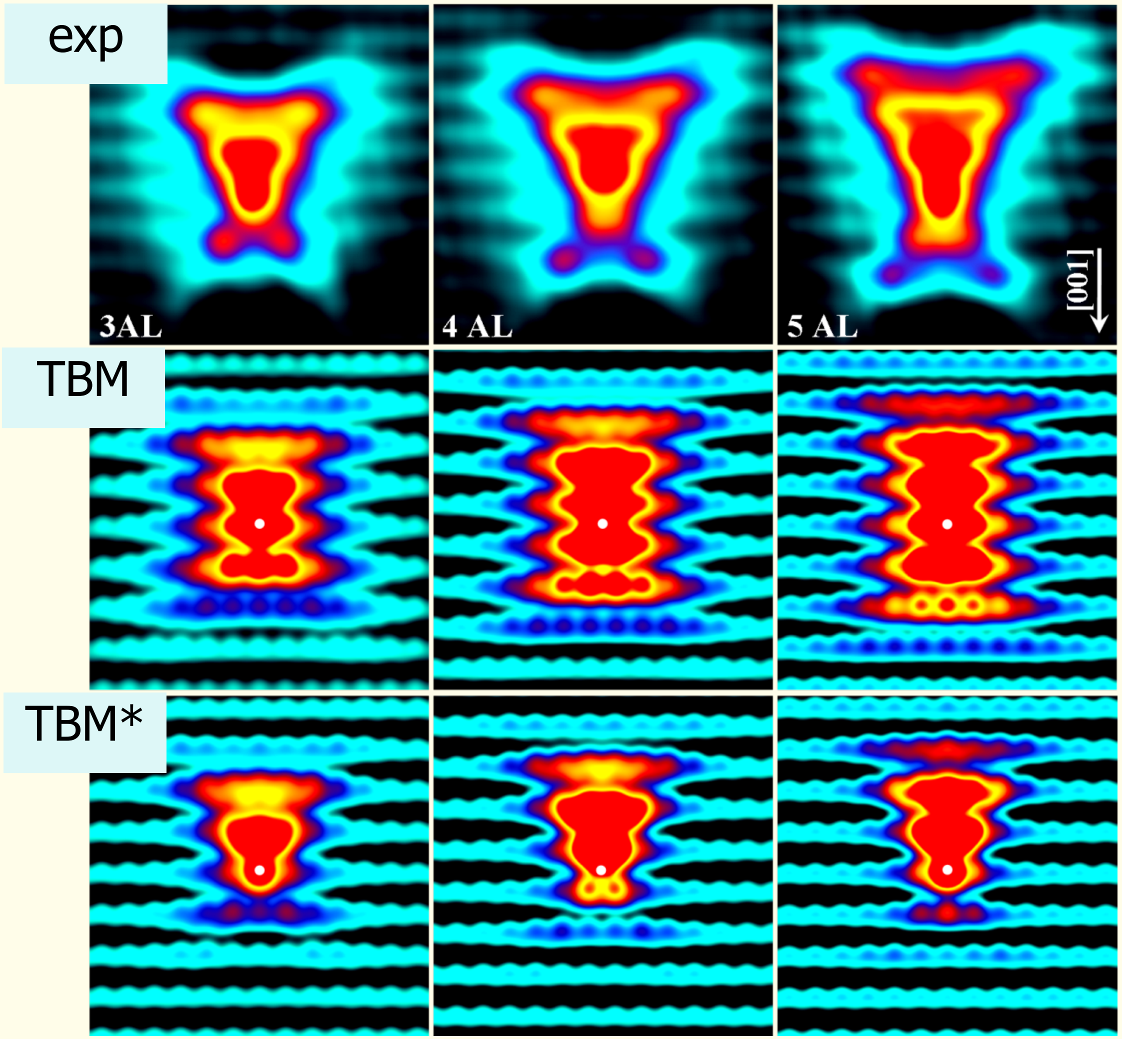
*J. Garleff et al PRB **78**, 075313 (2008)*

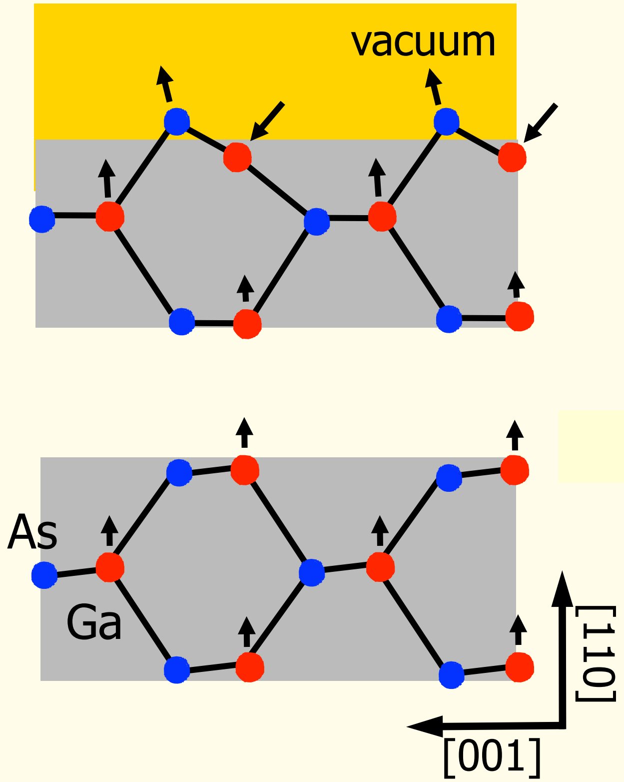
Strained Mn impurities



A. Yakunin et al, Nature Materials ***6****, 512 (2007)*

Effect of Surface relaxation





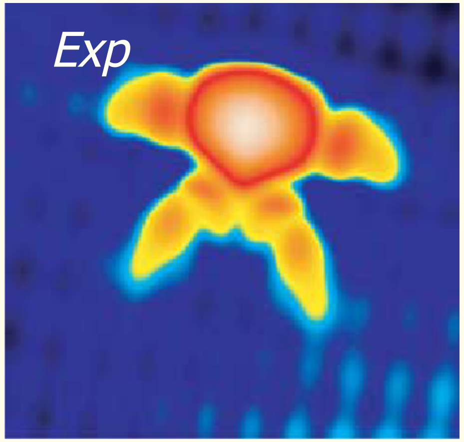
Ga sublattice shifted by 0.014 Ang in 110 direction (0.25 % of lattice constant)

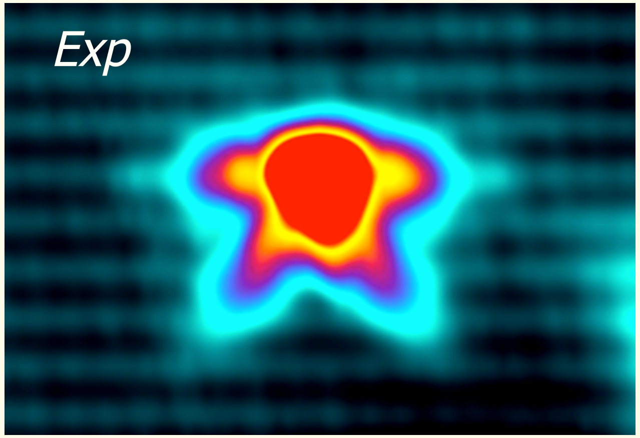
*Celebi et al PRL **104**, 086404 (2010)*

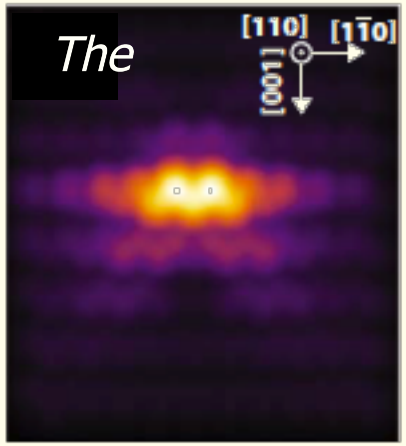
Mn Contrast

Kitchen et al., Nature ***442****, 436 (2006)*

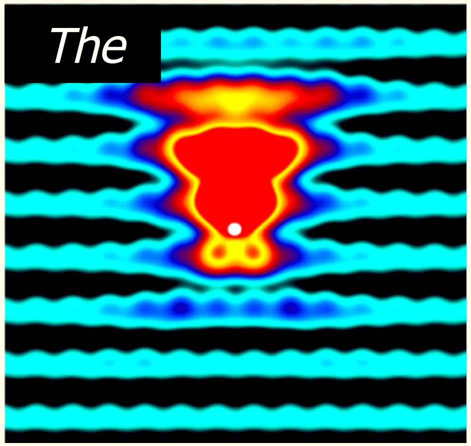
surface

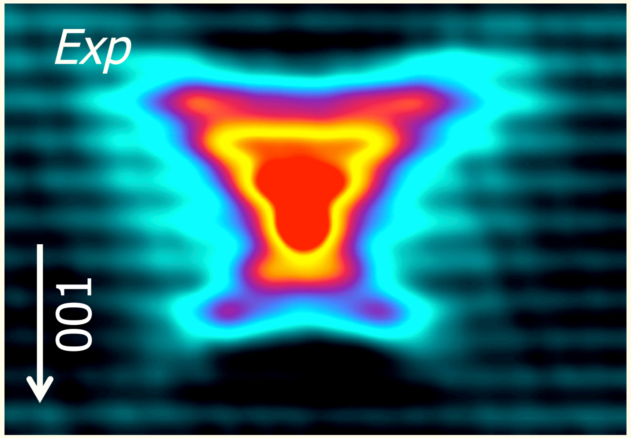


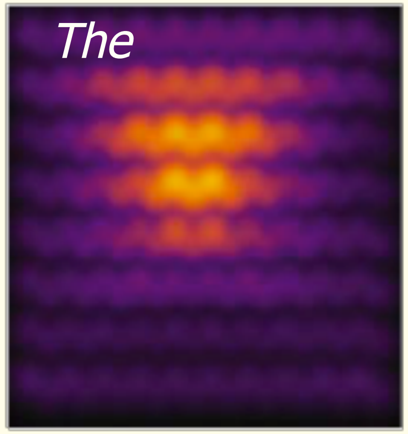




4th sublayer





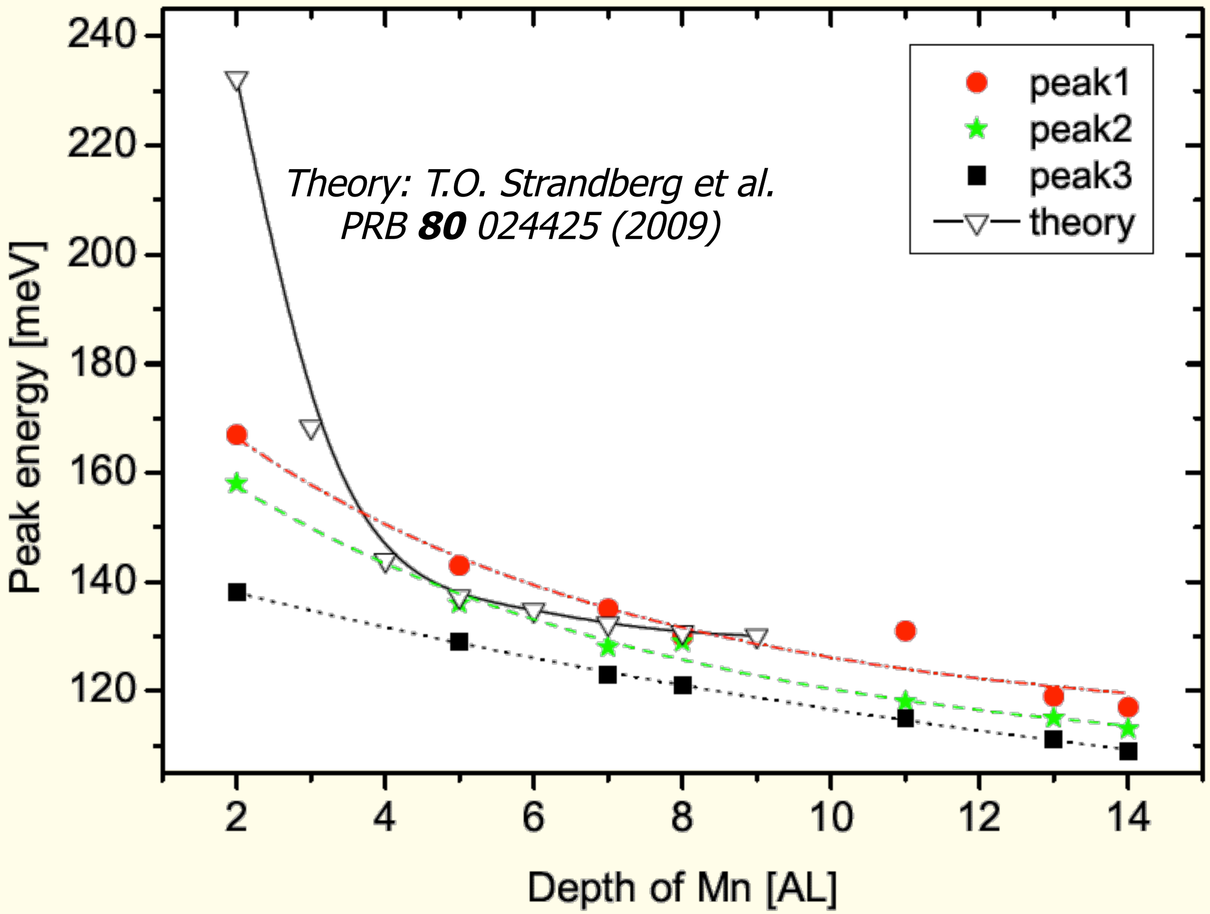


C. Celebi et al PRL ***104****, 086404 (2010)*

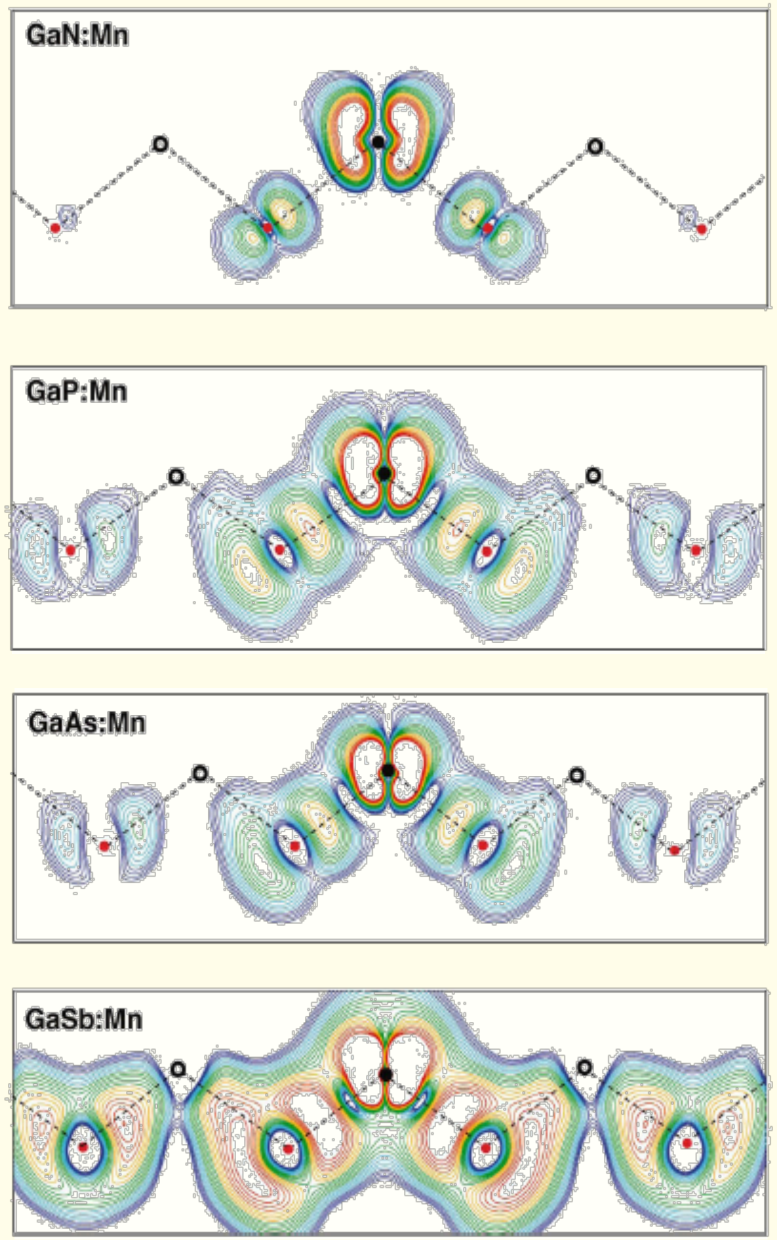
J. Garleff et al PRB ***78****, 075313 (2008)*

T.O. Strandberg et al. PRB ***80*** *024425 (2009)*

Binding Energy Mn Acceptor



*J. Garleff et al PRB **82** 035303 (2010)*



*P. Mahadevan and A. Zunger APL **85**, 2860 (2004)*

Shallow versus Deep Impurities

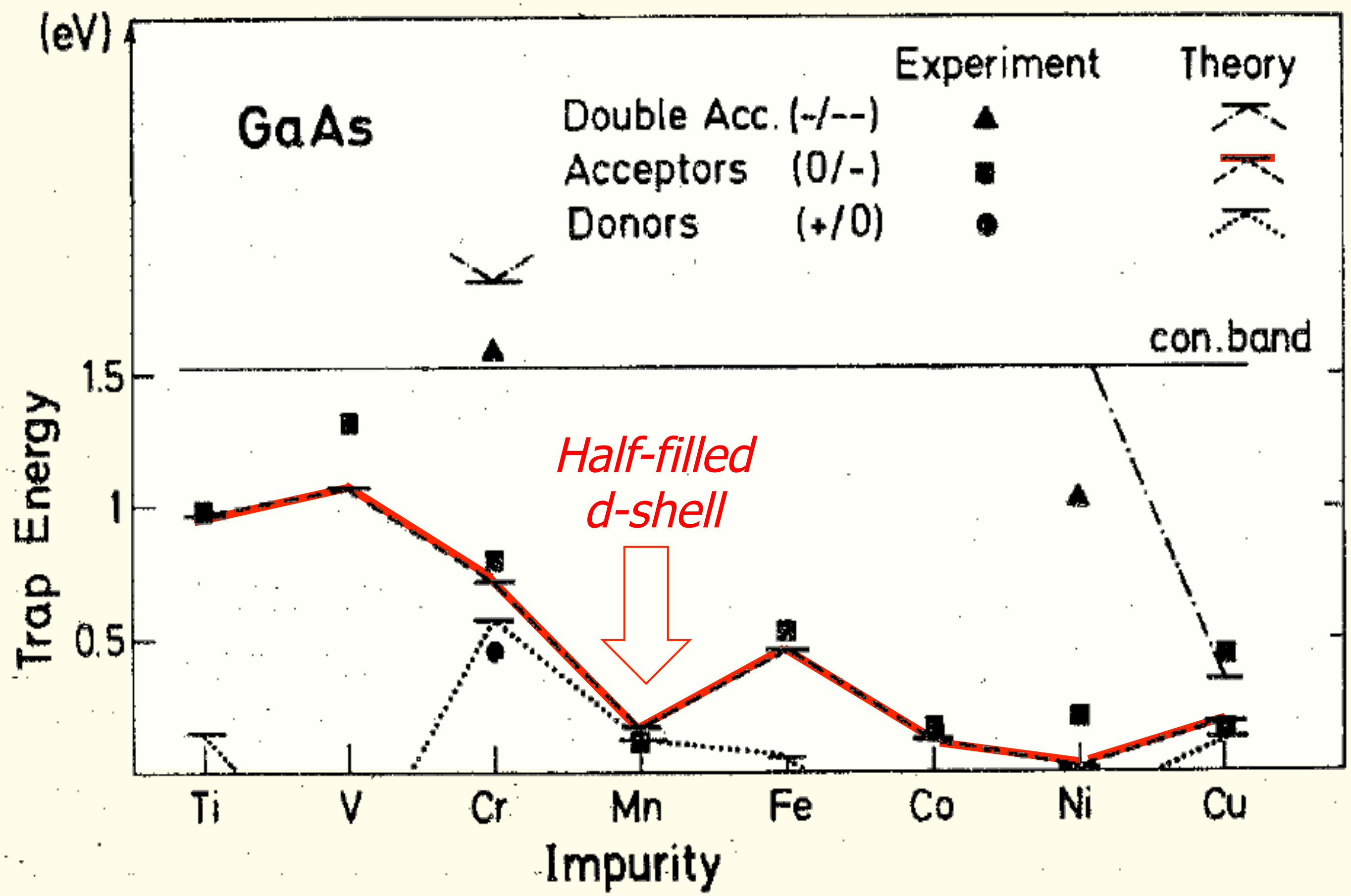
Shallow impurities

- *Long range confining potential mostly Coulombic (1/r)*
- *Effective mass modeling*
- *Large Bohr-radius, small binding energy*
- *Examples in GaAs: Si, Zn, Be, Sn*

Deep impurities

- *Atomic scale confining potential strongly non-Coulombic*
- *Advanced atomistic modeling*
- *Strongly localized, large binding energy*
- *Examples in GaAs: Fe, Cr, Er*

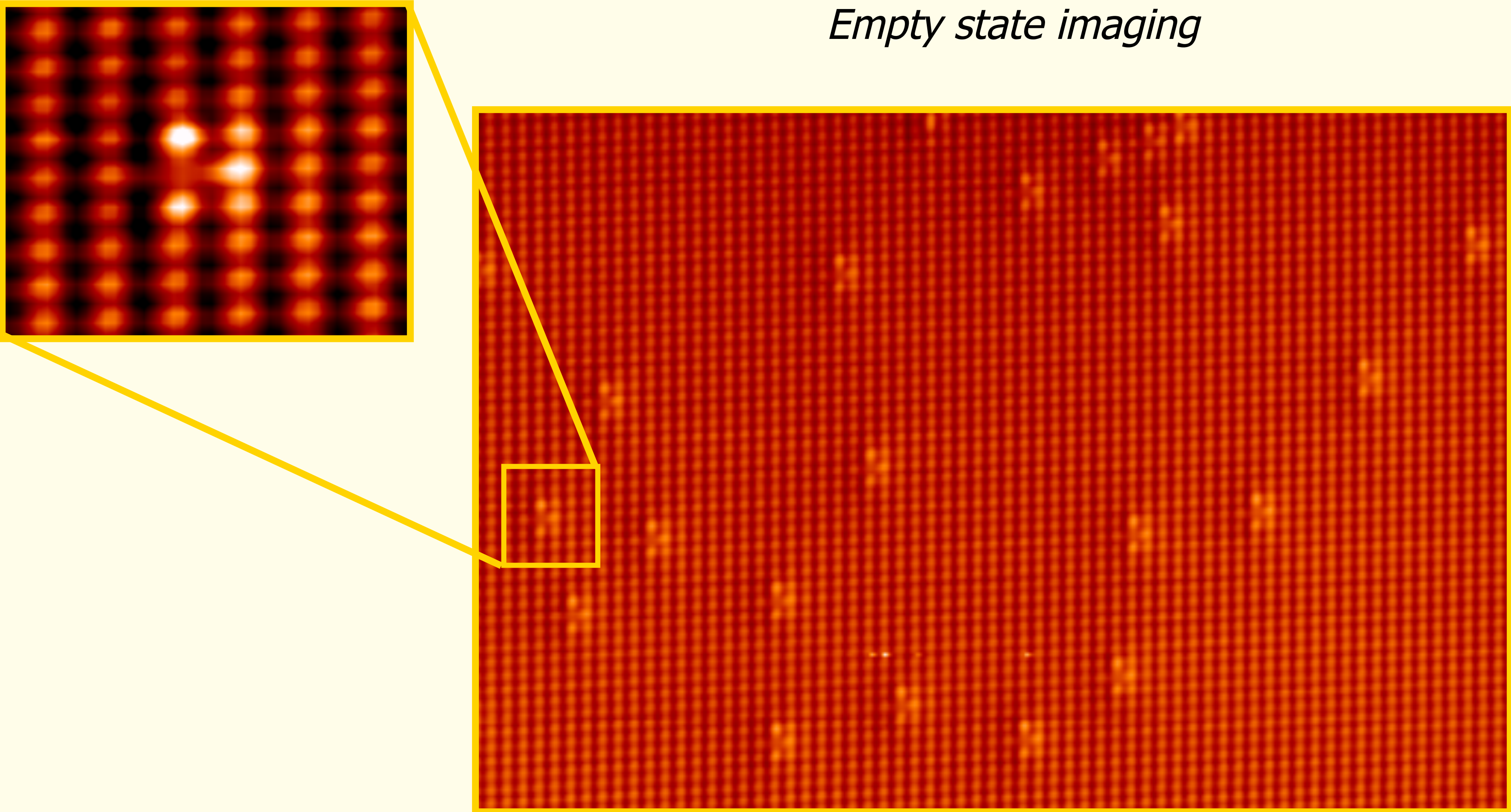
Transition Metal Impurities in GaAs



*P. Vogl and J.M. Baranowski, Acta Physica Polinica A **67**, 133 (1985)*

Cr doped GaP

Empty state imaging

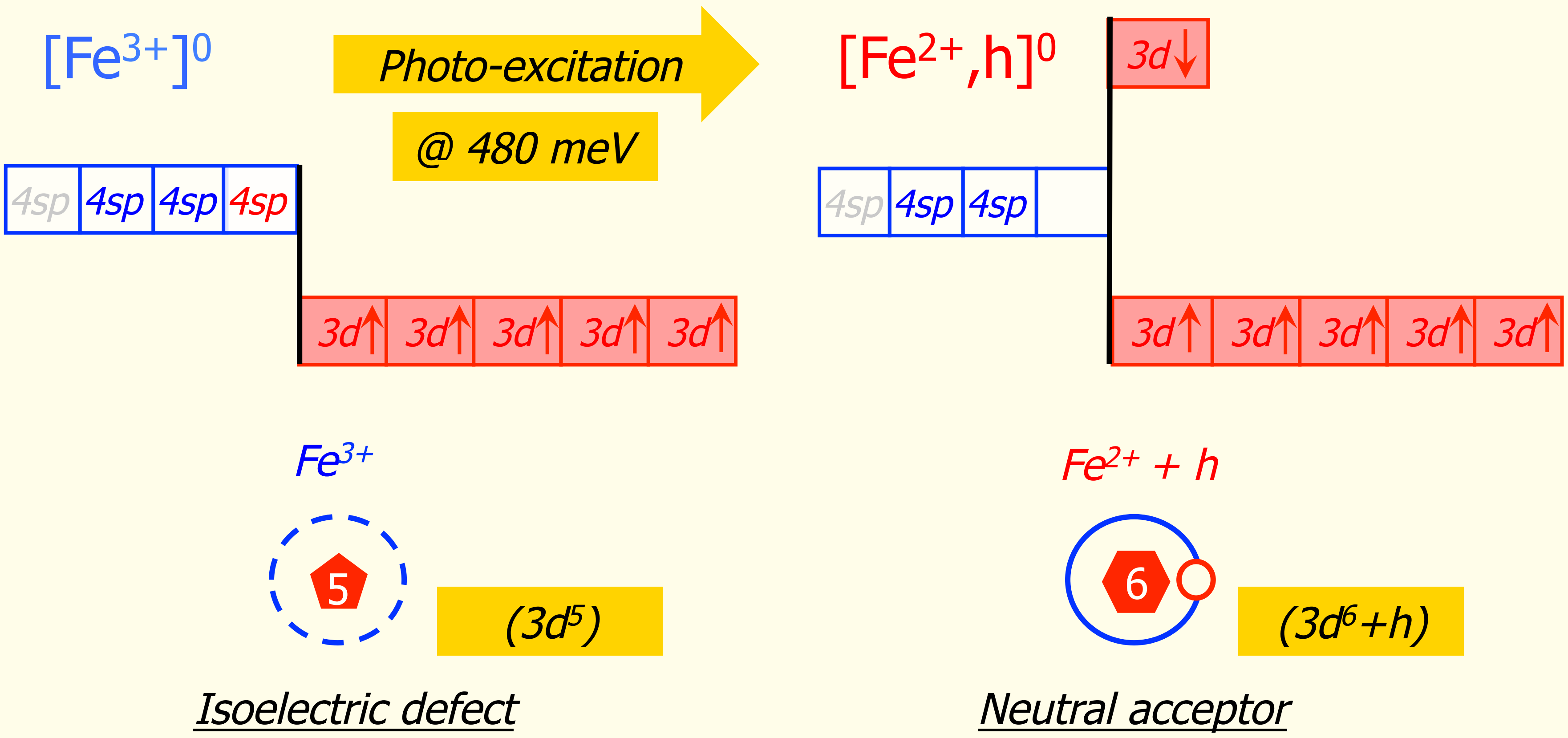


Artificial Atoms in Semiconductors

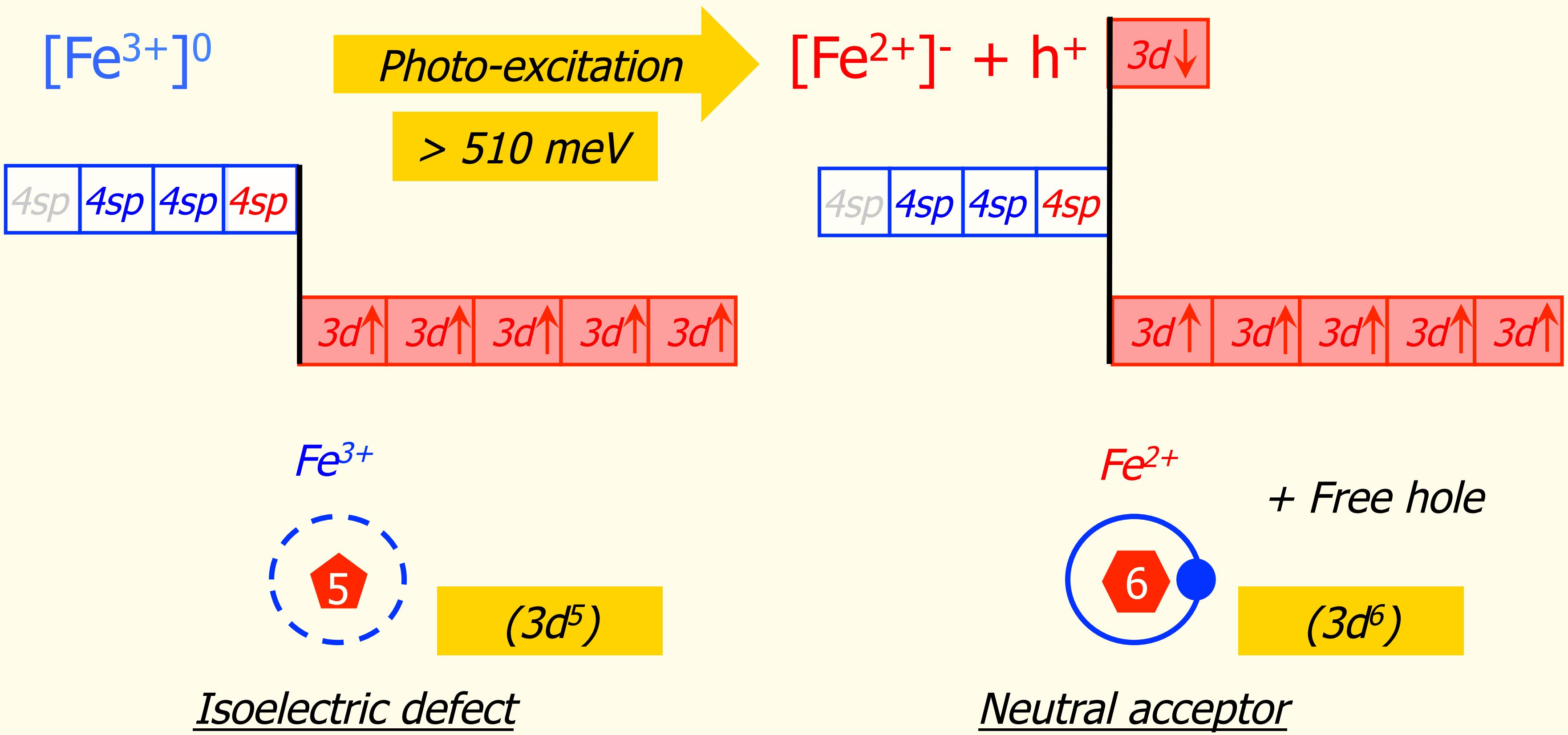
Outline

- ✓*Introduction*
- ✓*Analysis of individual donors in GaAs*
  - ✓*Charge manipulation (ionization)*
  - ✓*Electronic characterization*
  - ✓*Configuration manipulation (donor/acceptor)*
- ✓*Analysis of individual magnetic acceptors in GaAs*
  - ✓*Electronic characterization*
  - ✓*Valence state manipulation*
  - ✓*Magnetic characterization*
- ✓*Conclusions*

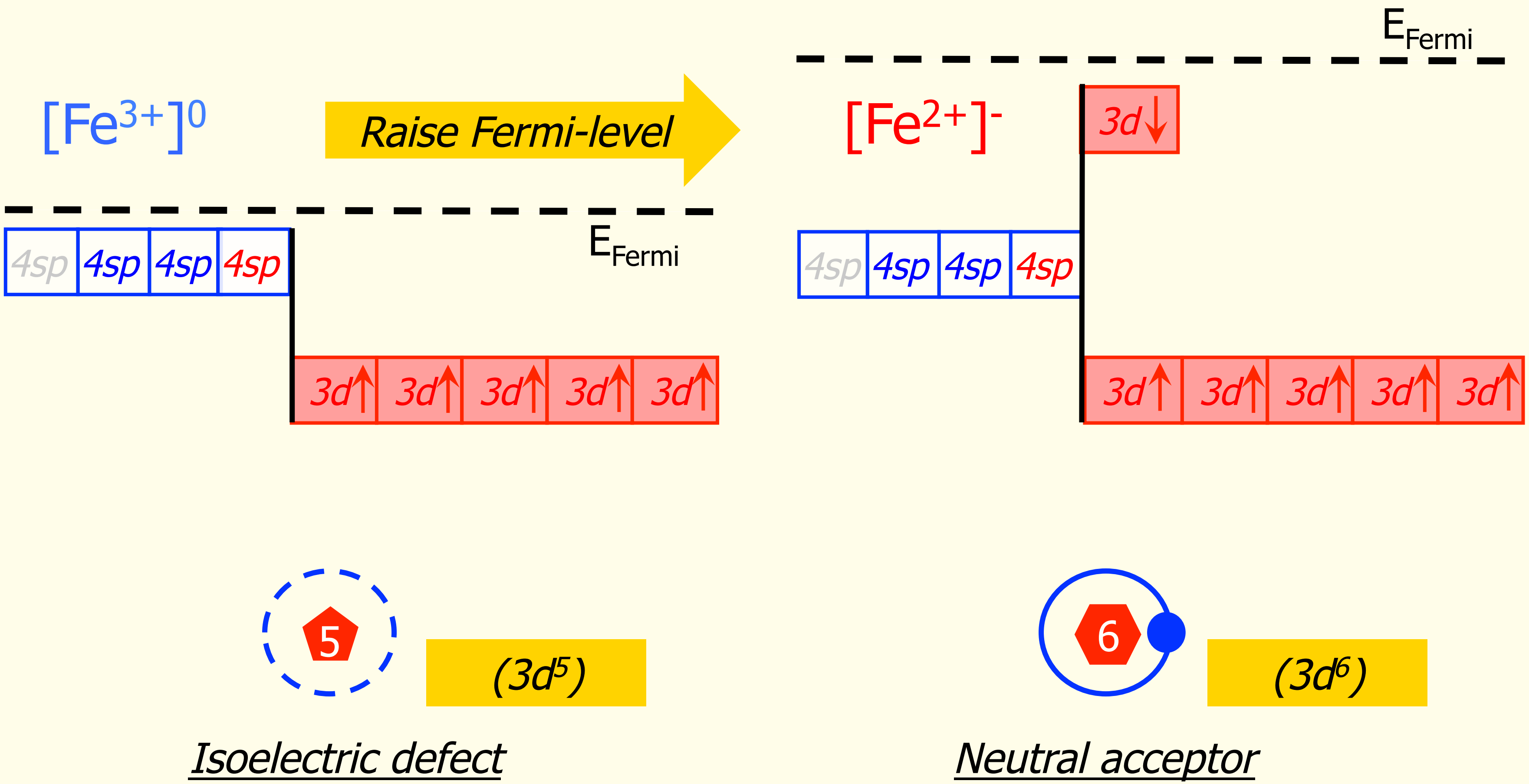
Electronic Structure Fe in GaAs



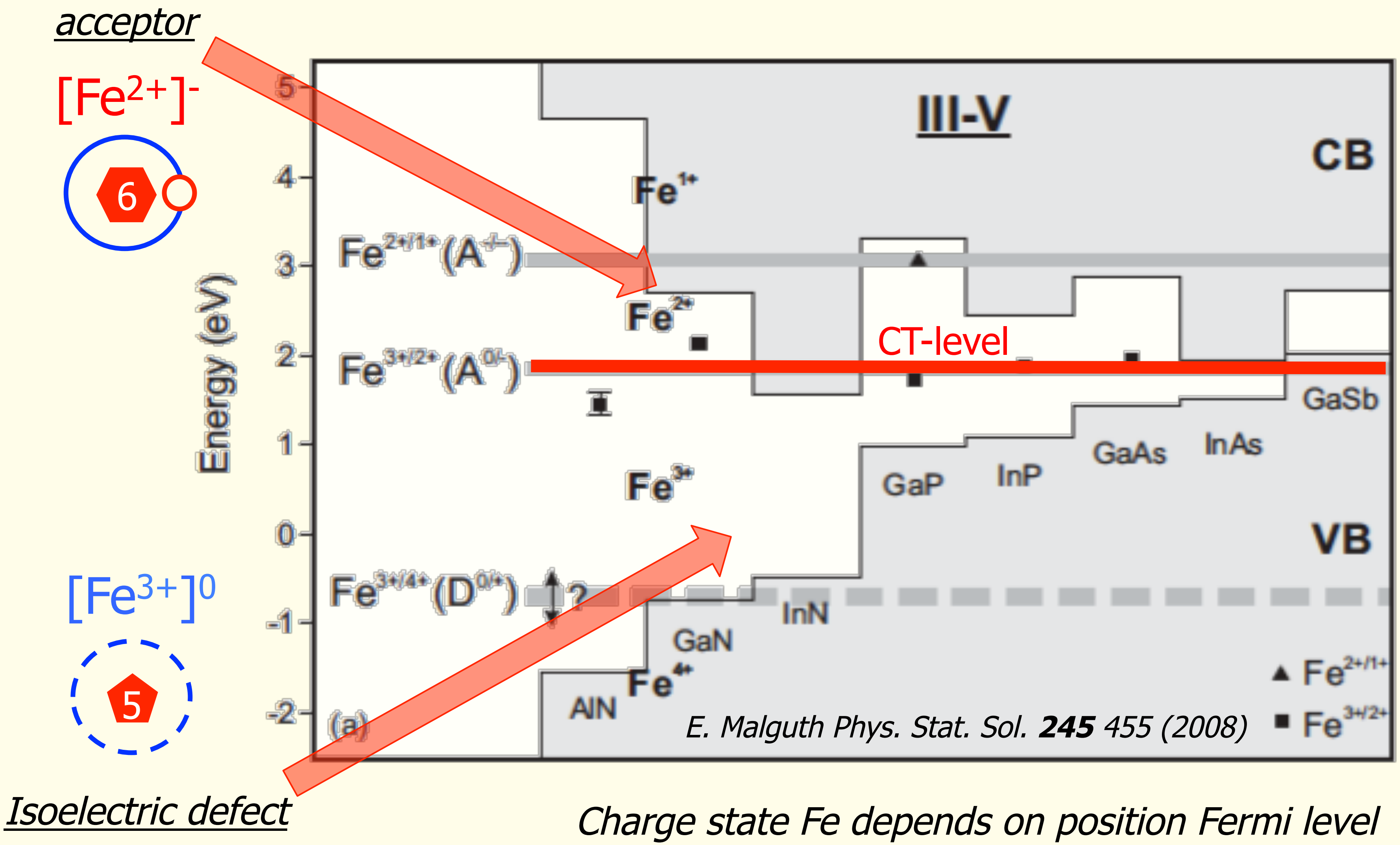
Electronic Structure Fe in GaAs



Electronic Structure Fe in GaAs

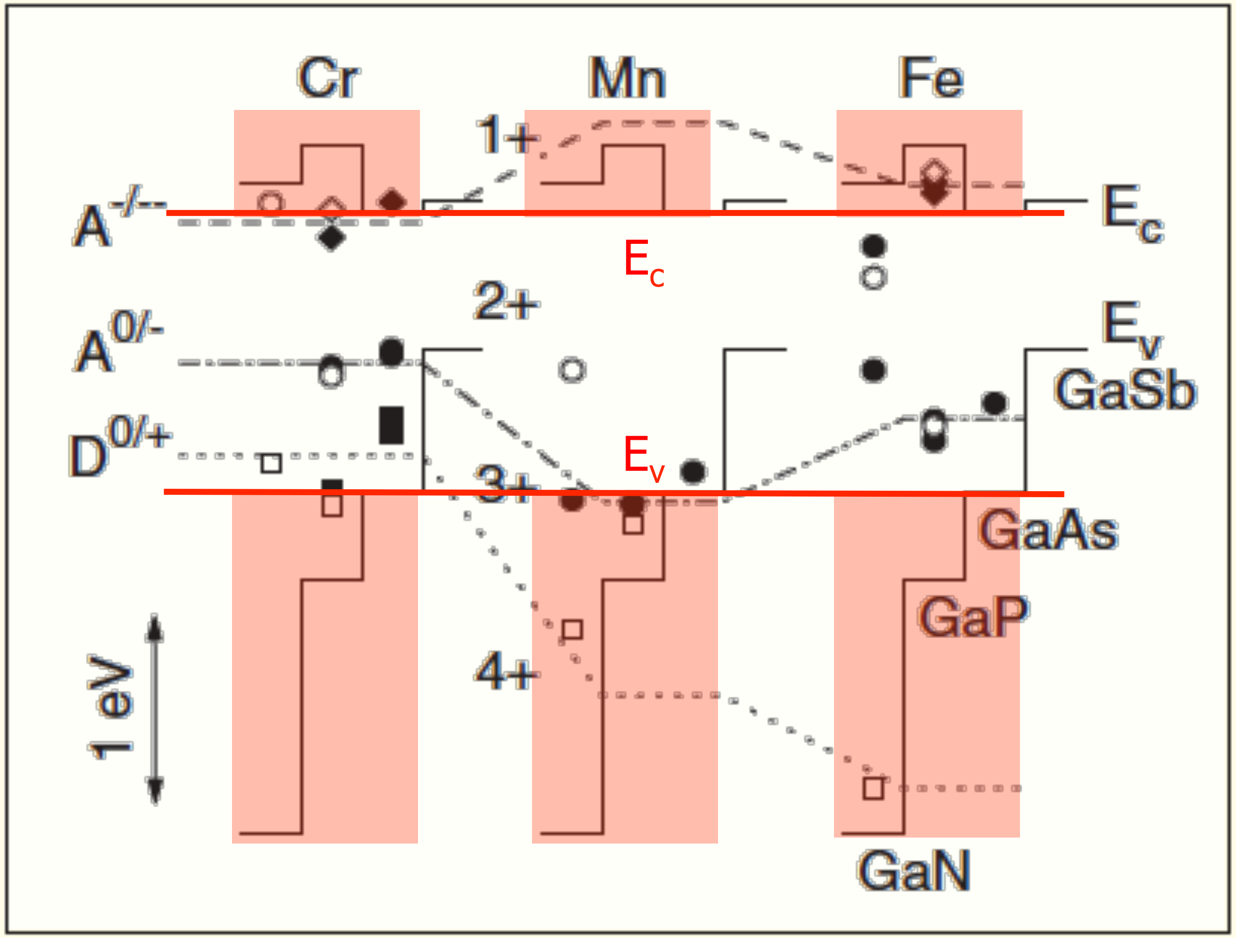


Charge Transfer Level Fe in III/V



Charge state Fe depends on position Fermi level

Transition Metal Impurities in GaAs

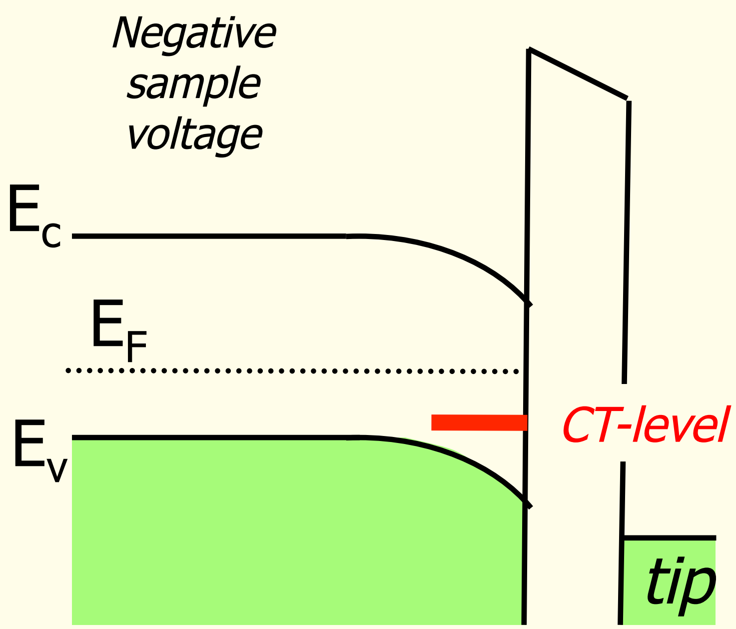


*T. Graf, S. Goennenwein, M. Brandt, Phys Status Solidi B **239**, 277 (2003)*

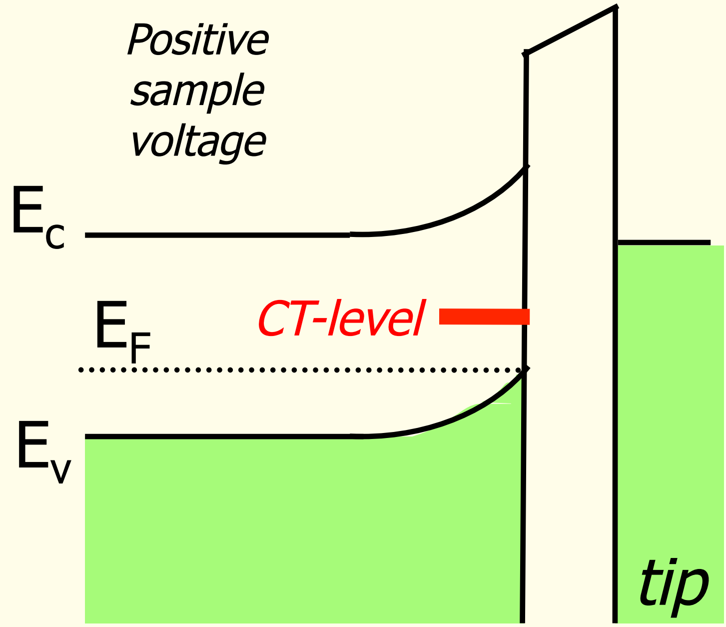
Manipulation of the Fe valence state

$[Fe^{2+}]^-$ *charged acceptor*

$[Fe^{3+}]^0$ *isoelectronic center*

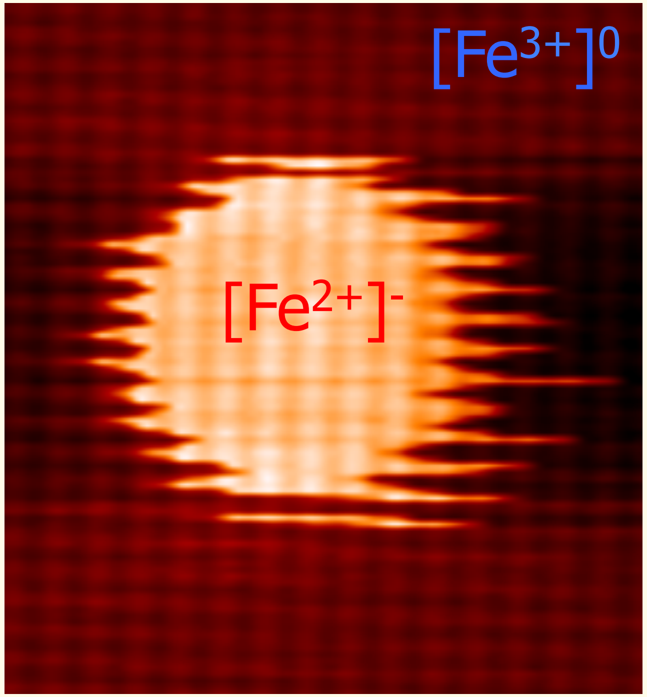


At large negative voltage ionized Fe^{2+}



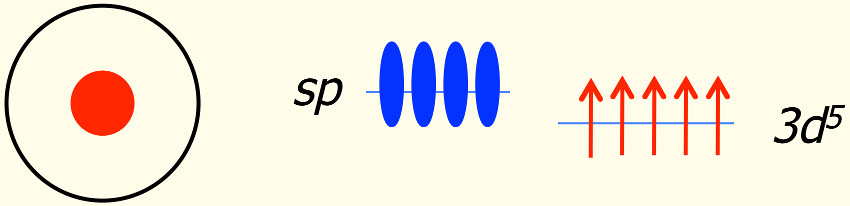
At large positive voltage neutral Fe^{3+}

Manipulation of Valence State of Fe by STM tip

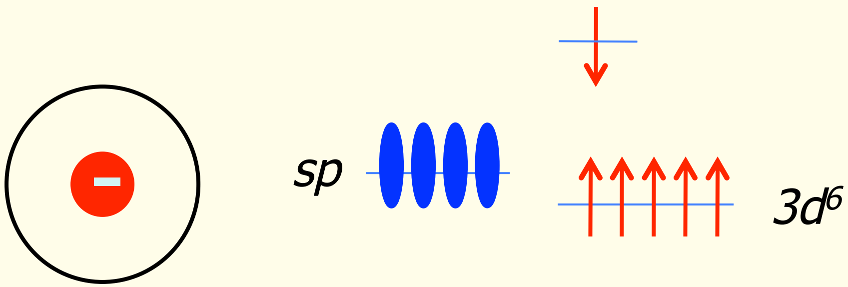


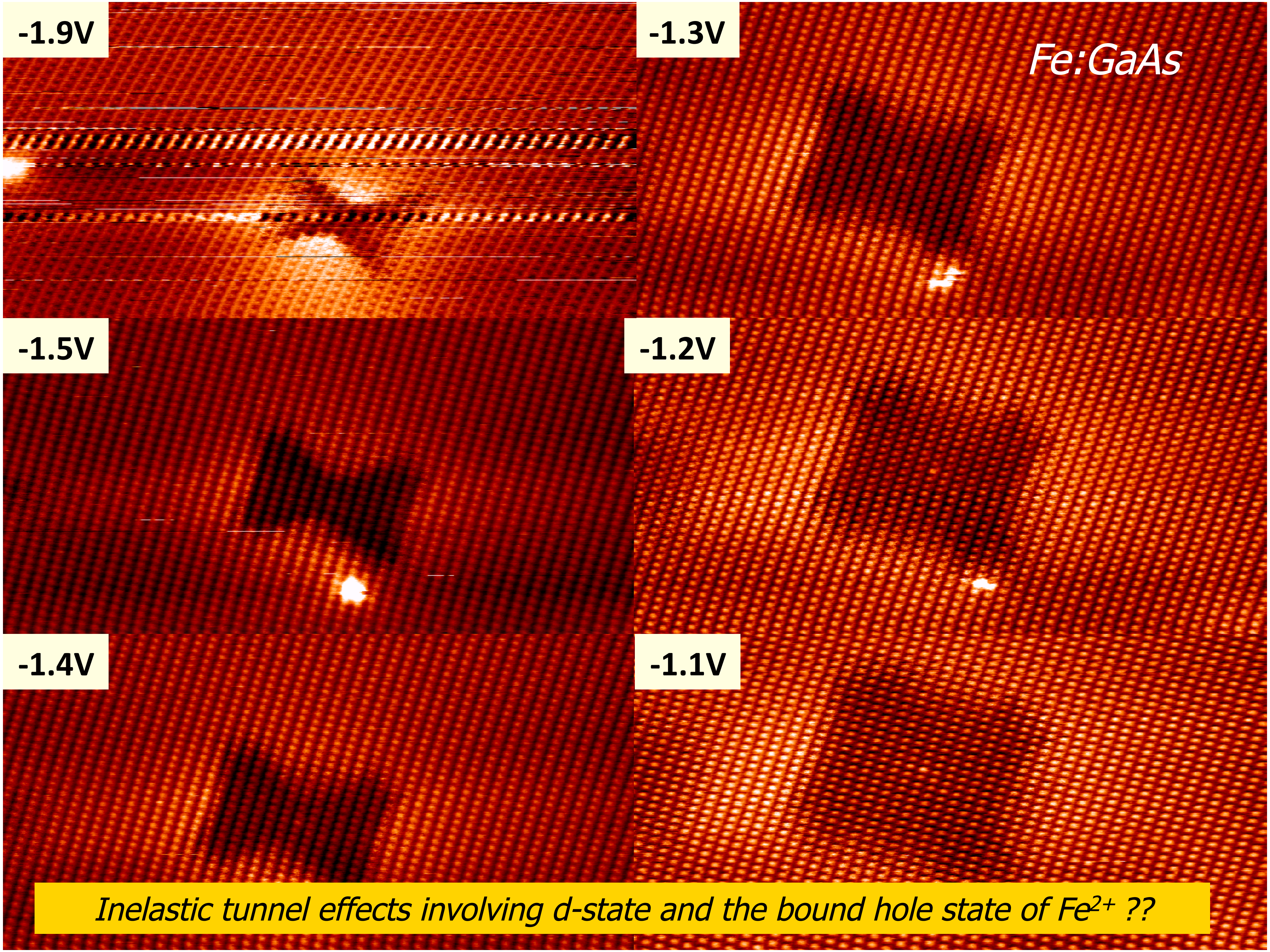
POSTER Juanita Bocquel (FP-47)

$[Fe^{3+}]^0$ *iso-electronic dopant*



$[Fe^{2+}]^-$ *ionized acceptor*





Inelastic tunnel effects involving d-state and the bound hole state of Fe^{2+} ??

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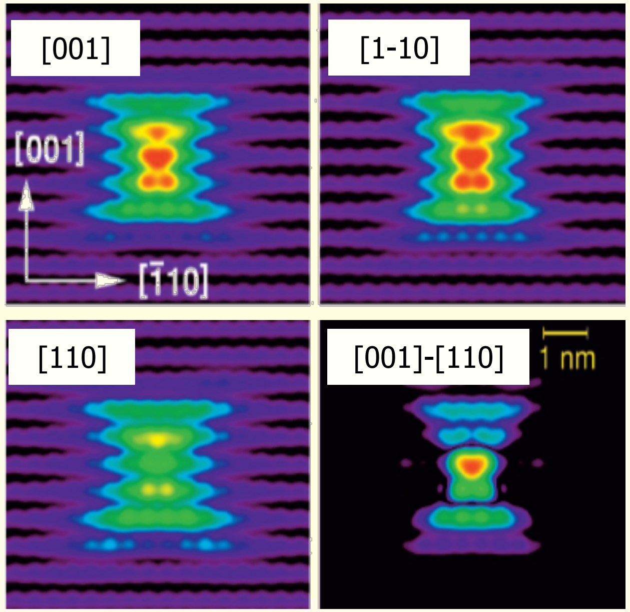
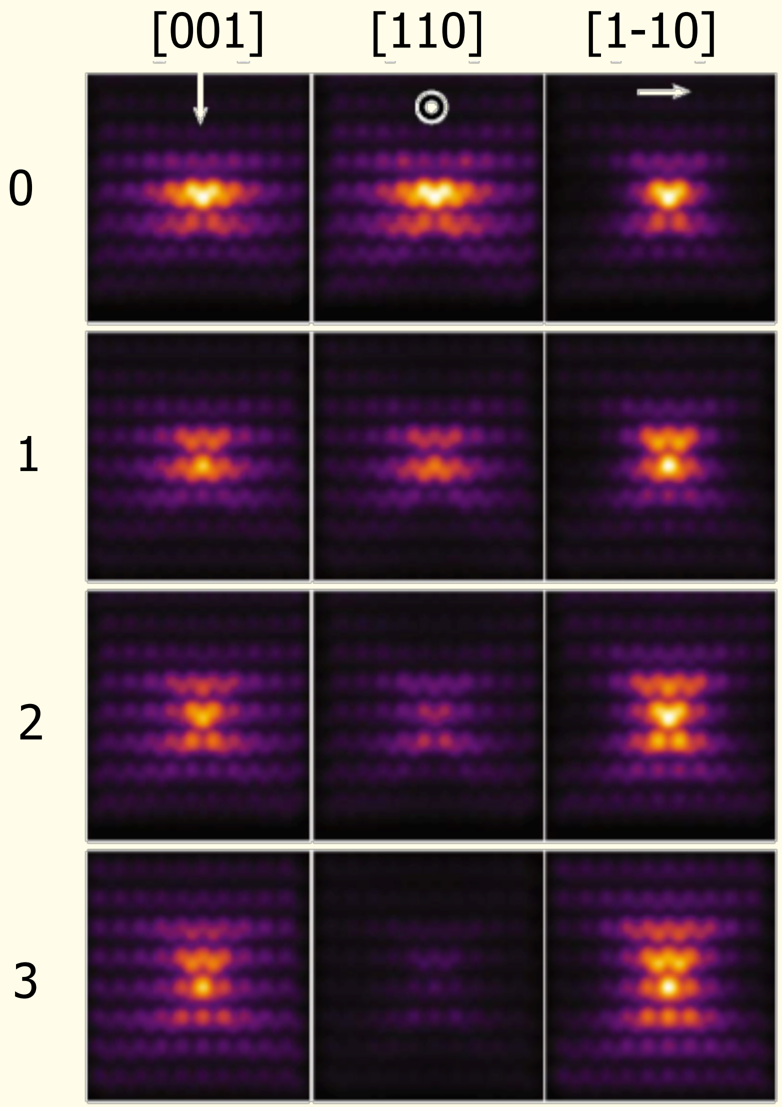
  - ✓ *Magnetic characterization*
- ✓ *Conclusions*

Magnetic Field Dependence

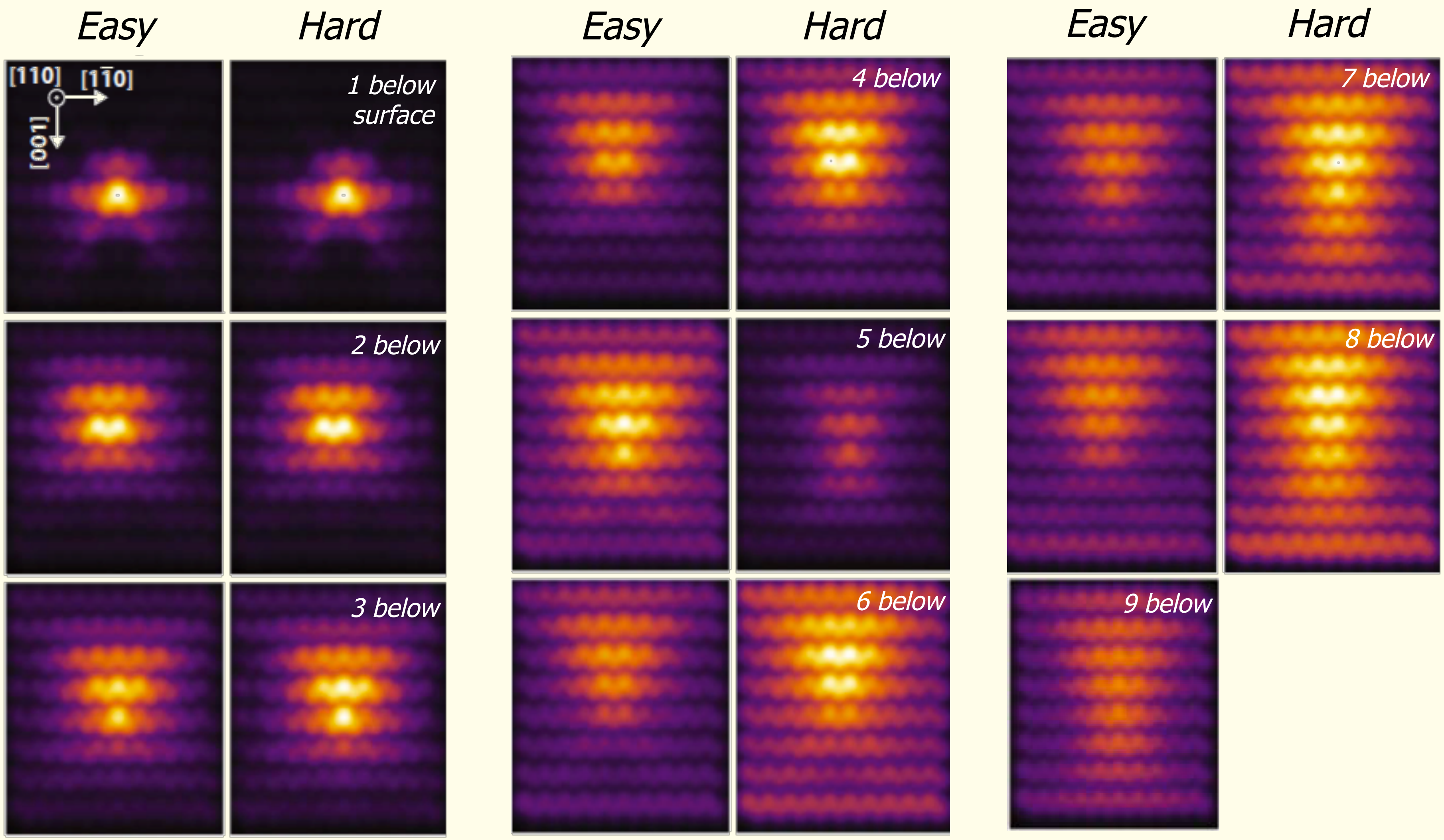


*Tang en Flatté, PRB **72**, 161315(R) (2005)*



*T.O. Strandberg et al. PRB **80** 024425 (2009)*

Depth Dependence Mn Contrast

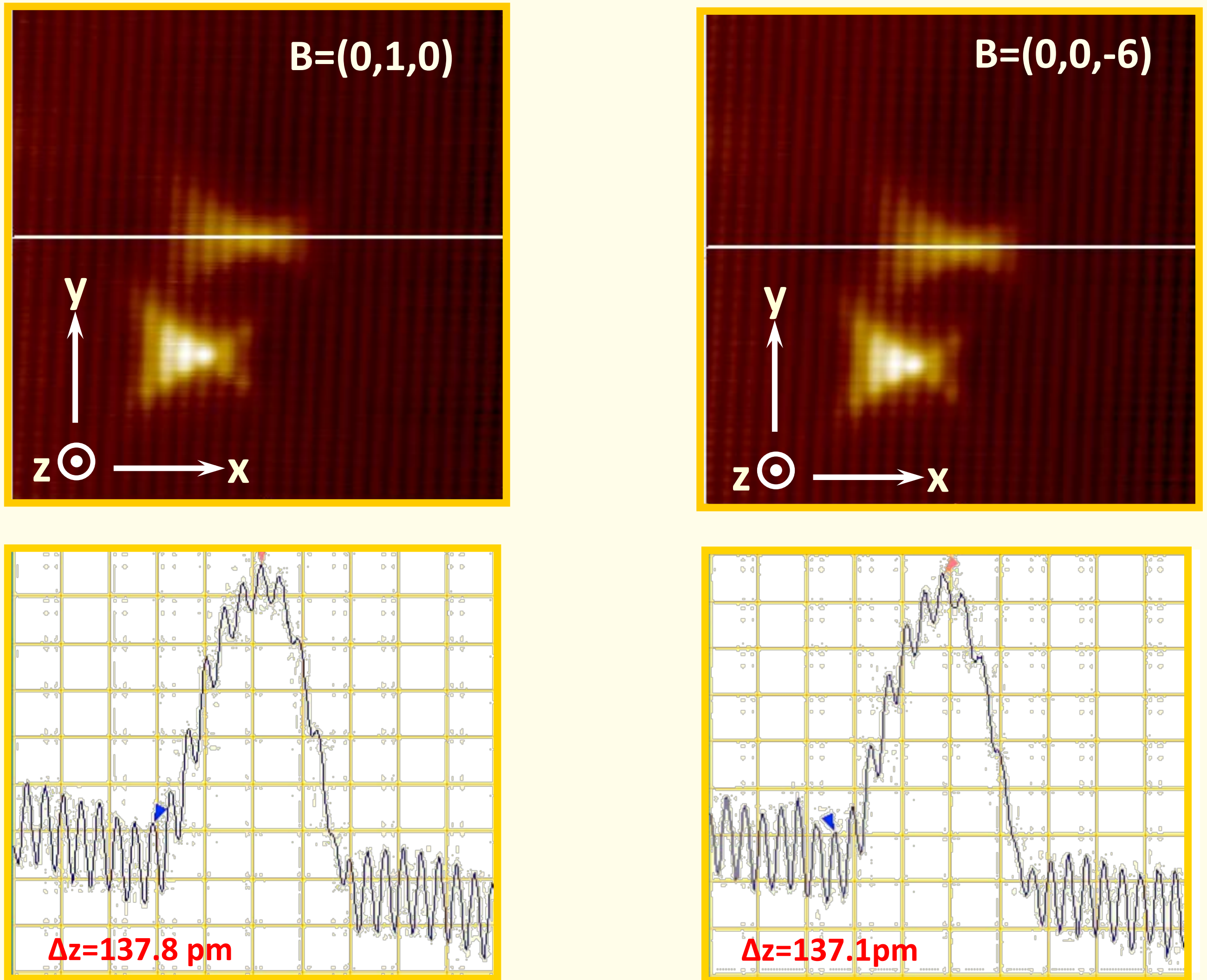


*T.O. Strandberg et al. PRB **80** 024425 (2009)*

Magnetic Field Dependence

Mn acceptor deep below surface

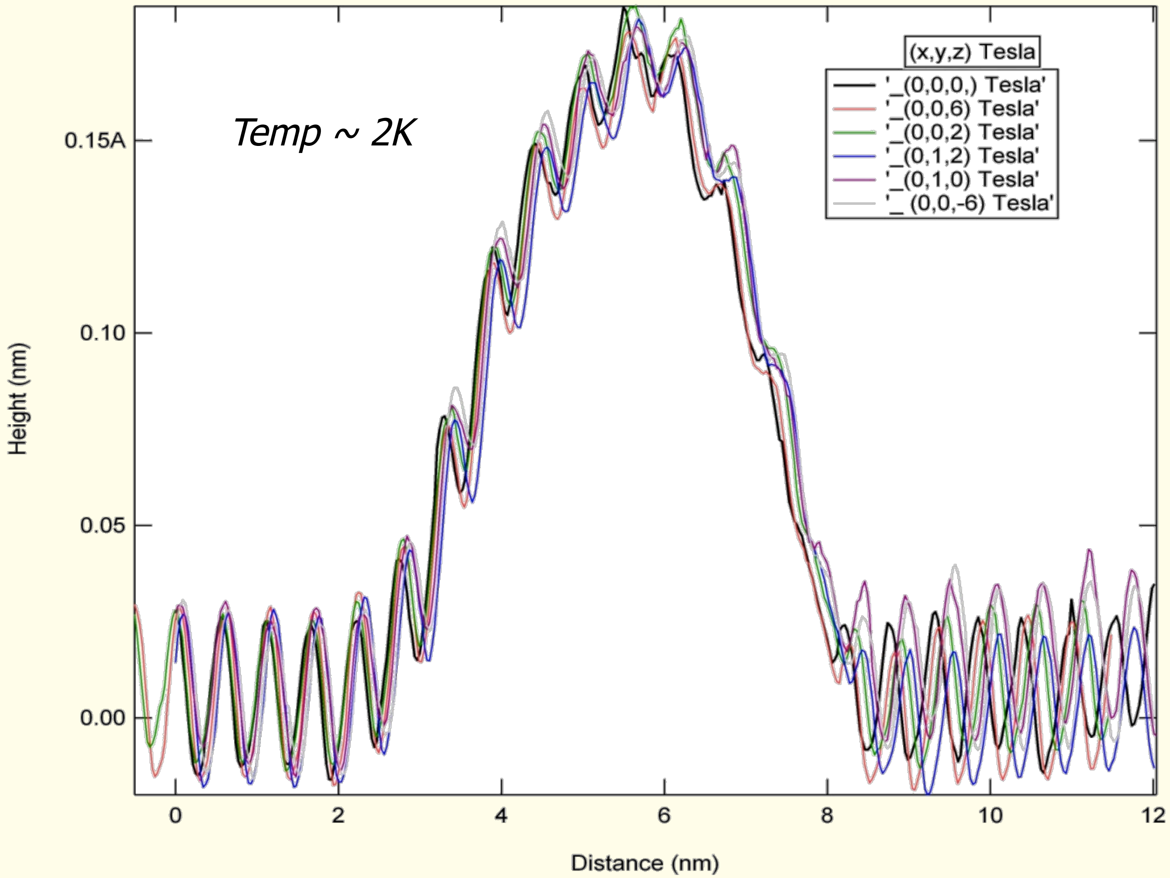
*26 nm * 26 nm*



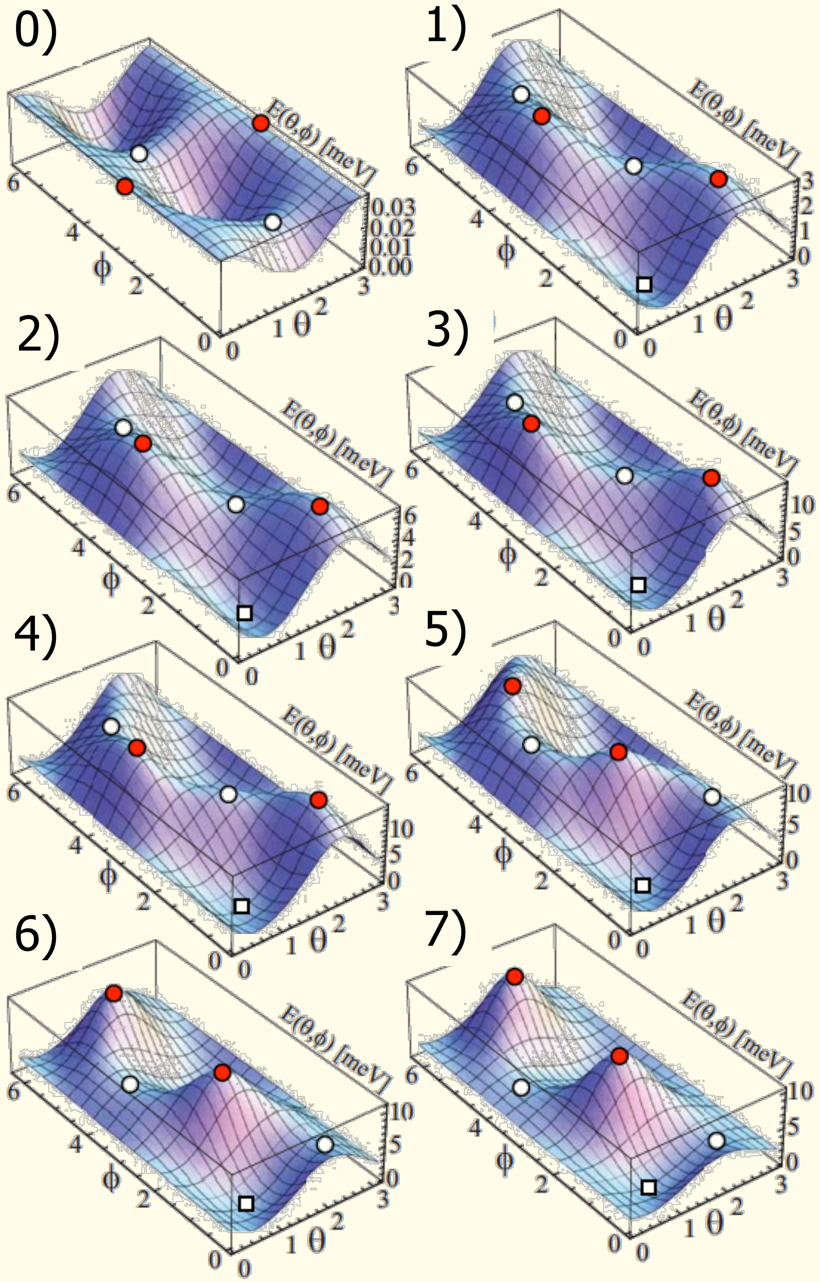
Temp ~ 2K

Magnetic Field Dependence

Mn acceptor deep below surface

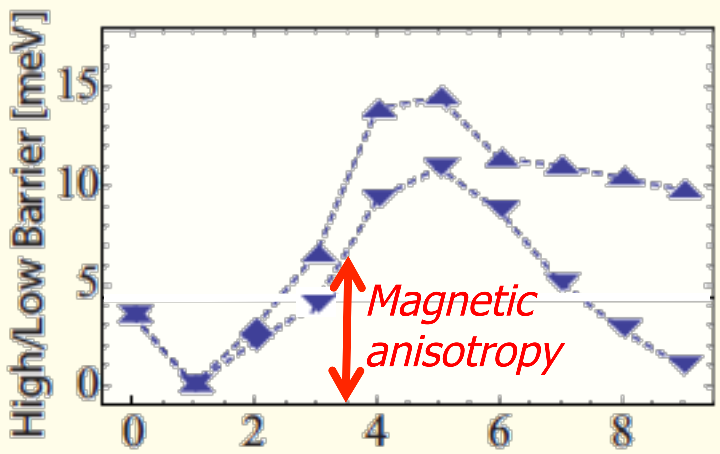


Magnetic anisotropy as function of depth below surface



Depth in ML below Surface

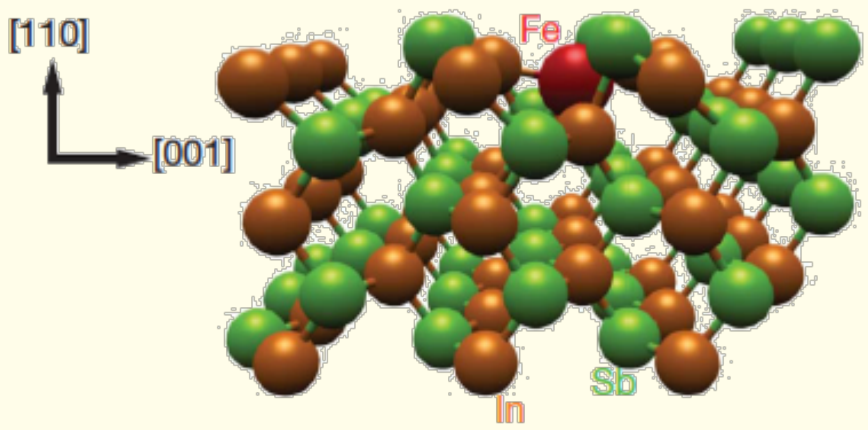
□ Minimal energy
○ Low barrier
● High barrier

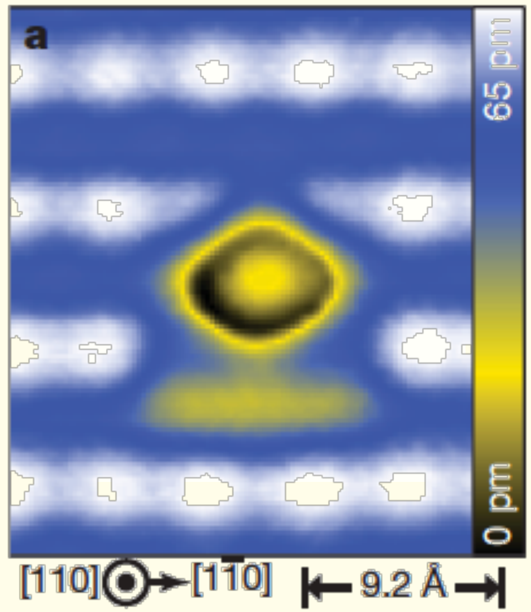


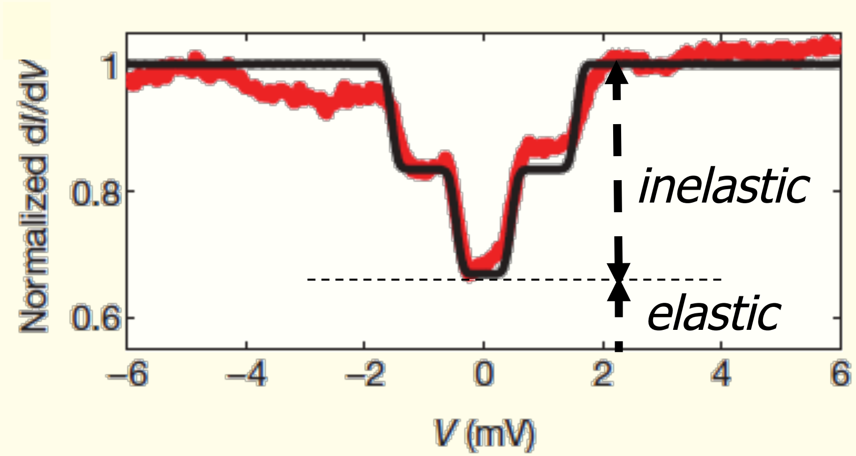
Depth in ML below Surface

*T.O. Strandberg et al, PRB **80** 024425 (2009)*

Spin Excitation of a Single Fe atom in an InSb Top-Surface Layer





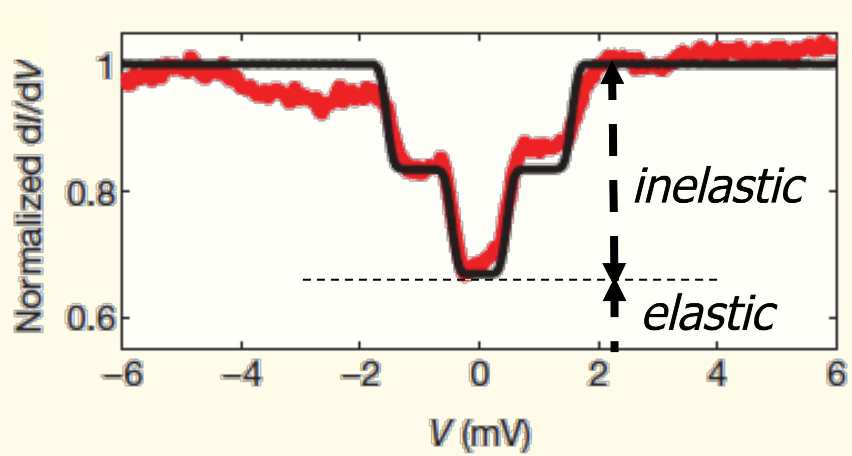


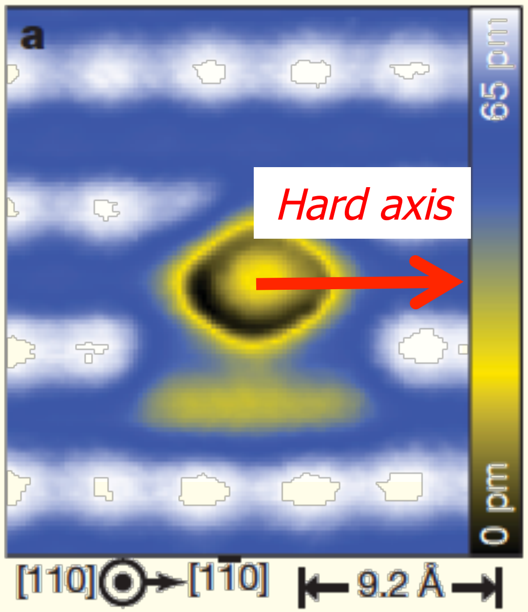
*A.A. Khajetoorians et al, Nature **467**, 1084 (2010)*

Spin Excitation of a Single Fe atom in an InSb Top-Surface Layer

$$H = D\hat{S}_z^2 + E\left(\hat{S}_x^2 - \hat{S}_y^2\right)$$

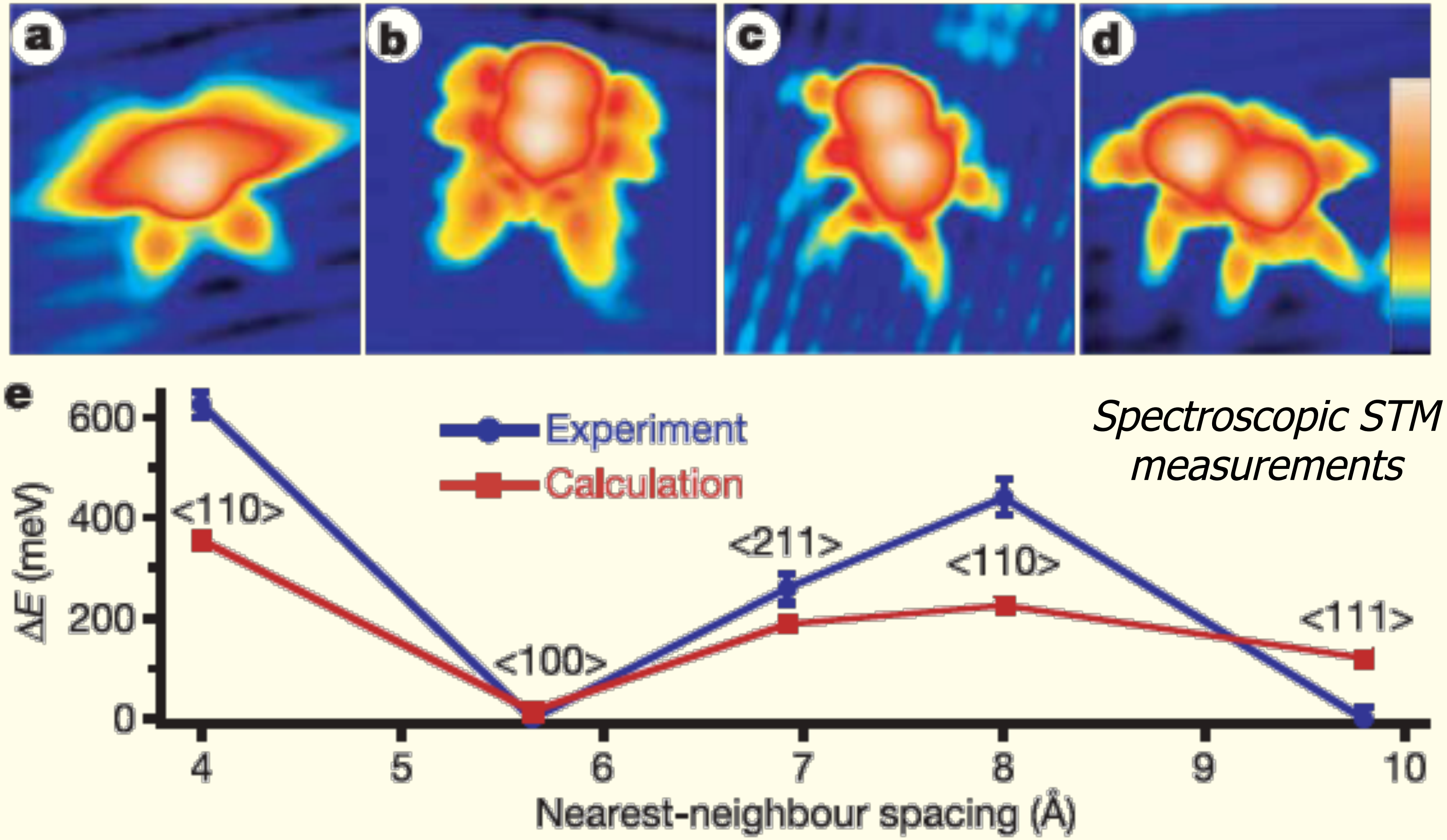
D = 0.75 meV *E = 0.5 meV*





*A.A. Khajetoorians et al, Nature **467**, 1084 (2010)*

Anisotropic Spin-Interaction for Mn in a GaAs Surface

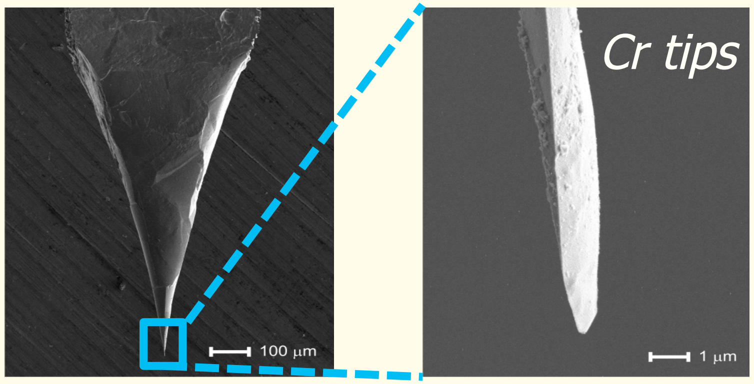


Spectroscopic STM measurements

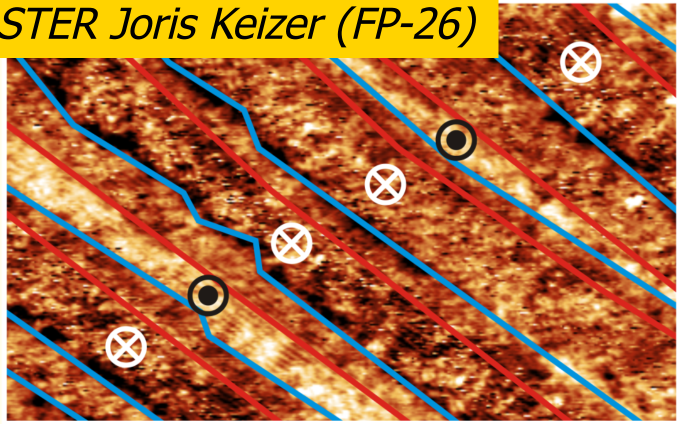
*D. Kitchen et al, Nature **442**, 436 (2006)*

Spin-Polarized Tunneling on Mn

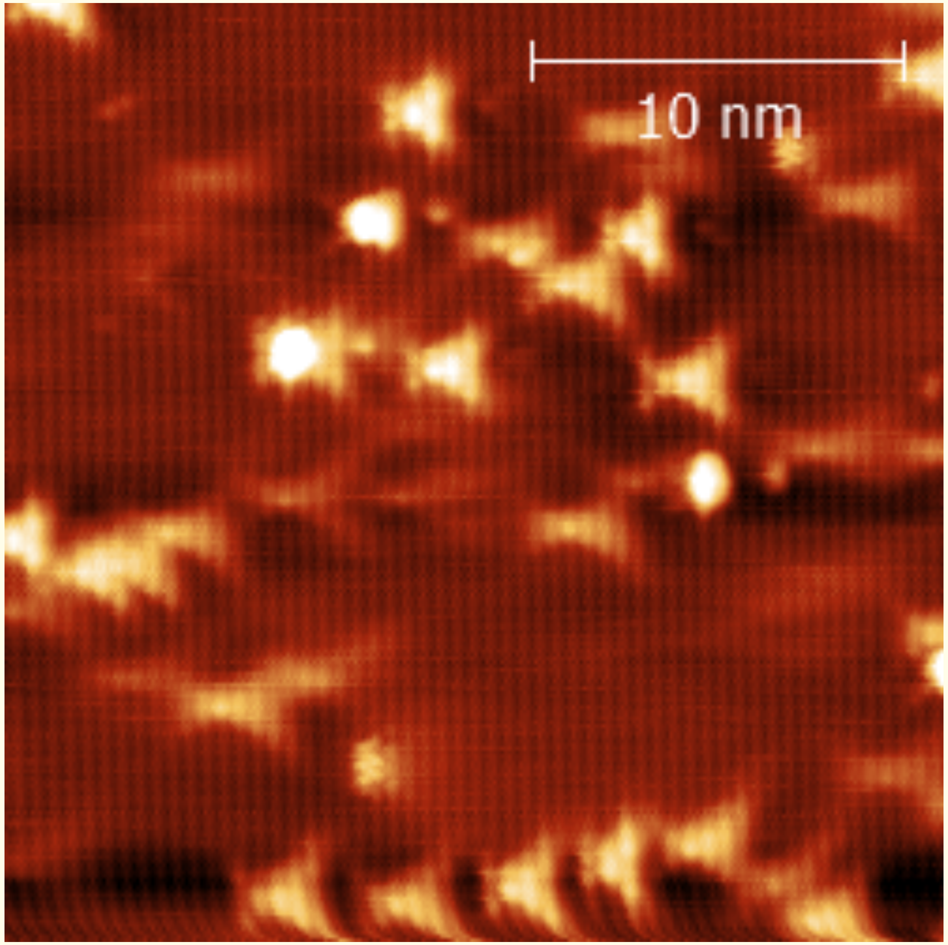
*Schlenhoff et al. APL **97**, 083104 (2010)*



POSTER Joris Keizer (FP-26)



out-of-plane magnetization observed on 1.5 ML Fe on W



Atomic resolution with Cr tip on Mn:GaAs

Collaborators

TU/e

J. Bocquel, M. Bozkurt, C. Celebi, J. Garleff, j. Keizer,
S. Mauger, A. Silov, A.Yakunin, I. Wijnheijmer

Experimental

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(University of Gottingen, Germany)
B. Bryant, N. Curzon, C. Hirjibehedin (UCL, London, UK)

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M.E. Flatté, C.E. Prior (University of Iowa, USA)
J.M. Tang (University of New Hampshire, USA)
A. Monakhov, N. Averkiev (Ioffe-institute, Russia)
M. Roy, P. Maksym (University of Leicester, UK)

Growers

W. Van Roy (IMEC-Leuven, Belgium)
B. Gallagher, R. Campion, V. Grant, T. Foxon (Nottingham, UK)
E. Marega (San Carlos, Brazil) & G. Solomon (Arkansas, USA)

What did Pauli have to say about semiconductor surfaces?

"One shouldn't work on semiconductors, that is a filthy mess; who knows whether any semiconductors exist."

Wolfgang Pauli
(1900-1958)

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*Review on single dopant physics and devices, Nature Materials **10**, 91 (2011)*

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Review on single dopant physics and devices, Nature Materials ***10****, 91 (2011)*

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Review on single dopant physics and devices,
Nature Materials ***10****, 91 (2011)*

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Eindhoven

5-9 August 2012

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