Mn in GaAs: from a single impurity to ferromagnetic layers

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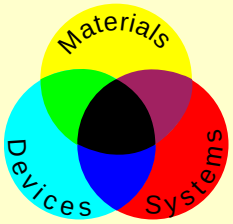


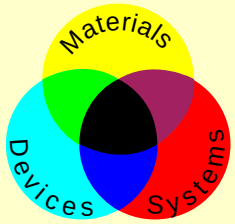
COBRA Inter-University Research
Institute on Communication Technology

KITP, 17 April 2006

Mn in GaAs: from a single impurity to ferromagnetic layers

Outline

- ✓ *Introduction*
- ✓ *Single impurities*
- ✓ *Symmetry breaking*
- ✓ *Coupled impurities*
- ✓ *Delta doping layers*



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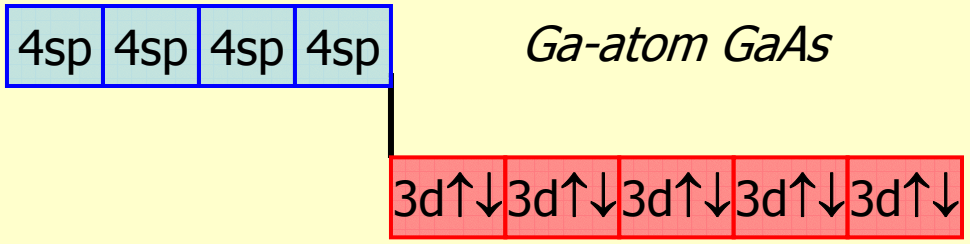
Albuquerque, 16 July 2005

Mn-Doping Atoms

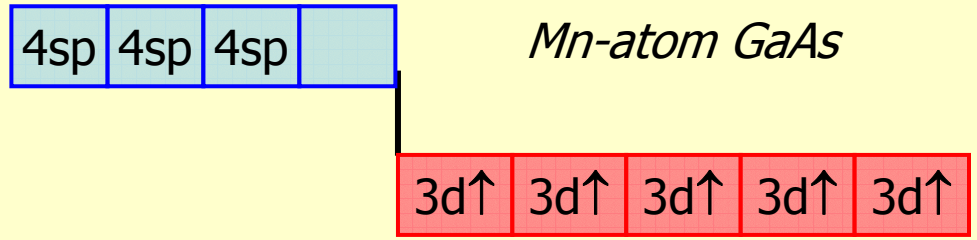
Electronic Structure

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



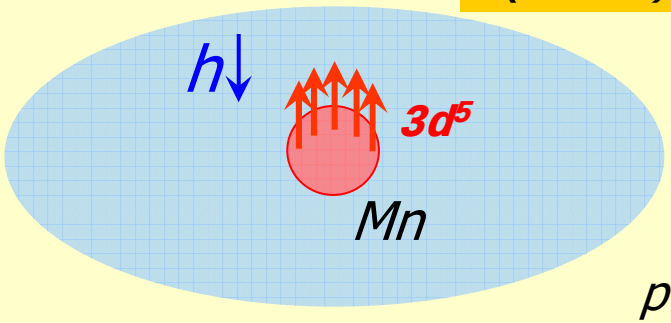
Ga-atom GaAs

Mn on Ga-site in GaAs



Mn-atom GaAs

$(3d^5+h)$



p-d interaction results in anti-ferromagnetic alignment

Electronic Structure

Anti-bonding (bound acceptor state)

States with Γ_{15} symmetry split due to SO interaction

Valence band states GaAs

4sp	4sp	4sp	4sp

Mn-atom in GaAs

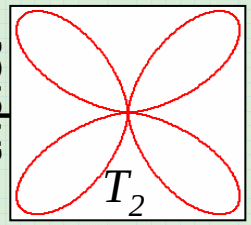
3d↑	3d↑	3d↑	3d↑	3d↑

Impurity band resonant with the valence band

113 meV ground state populated at T=0 when in neutral condition

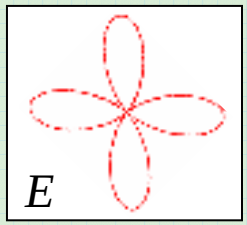
d-states split by cubic crystal symmetry

triplet



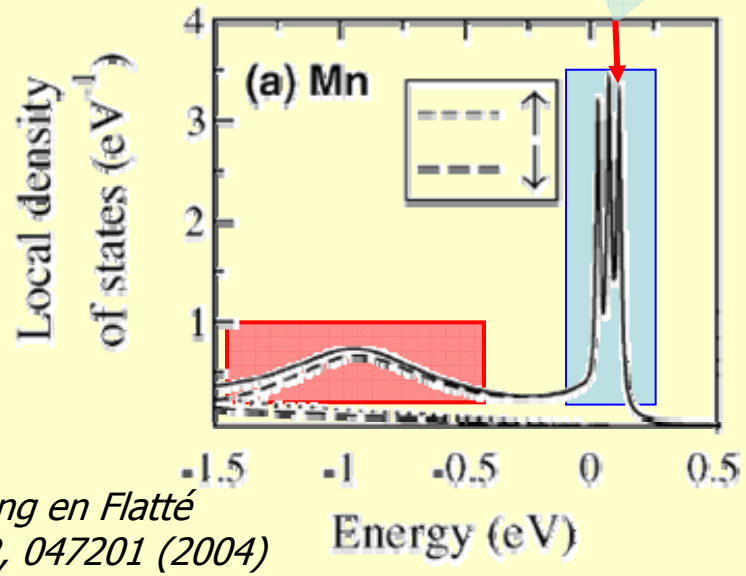
Γ_{15}

doublet



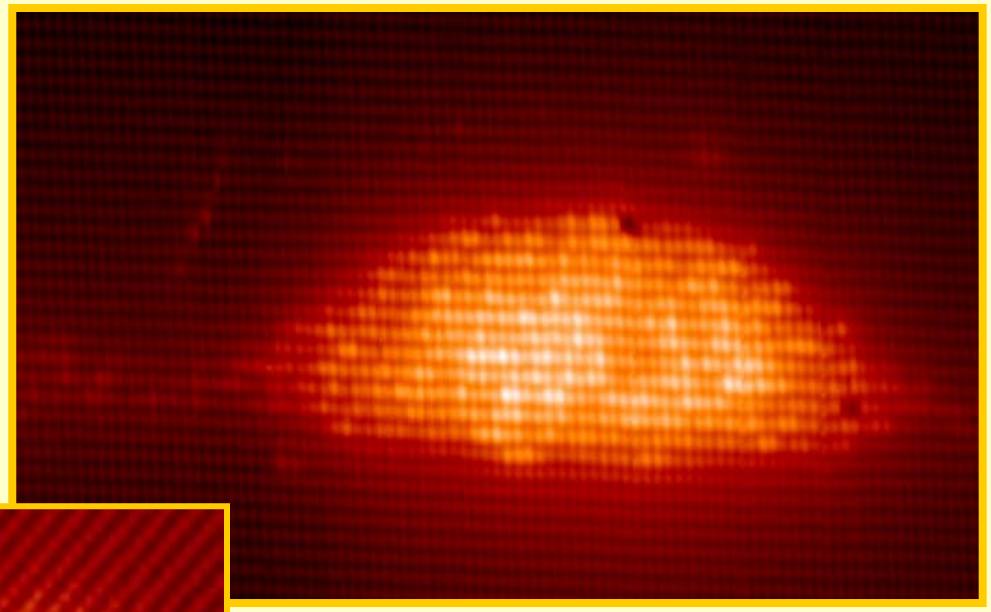
Γ_{12}

The p-d coupling to is strongest for d-states with Γ_{15} symmetry



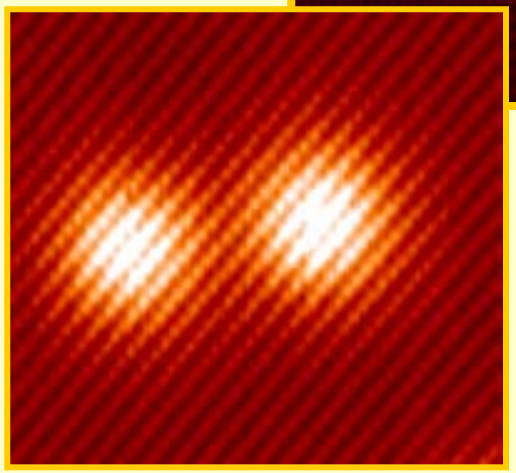
Tang en Flatté
*PRL **92**, 047201 (2004)*

Assessment at the Atomic Scale by Cross-Sectional STM



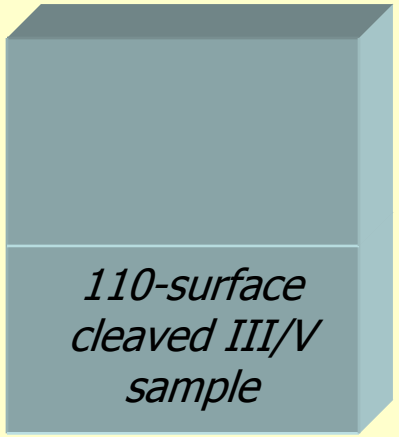
*15 nm * 30 nm*

InAs self-assembled quantum dot in GaAs



*9 nm * 8 nm*

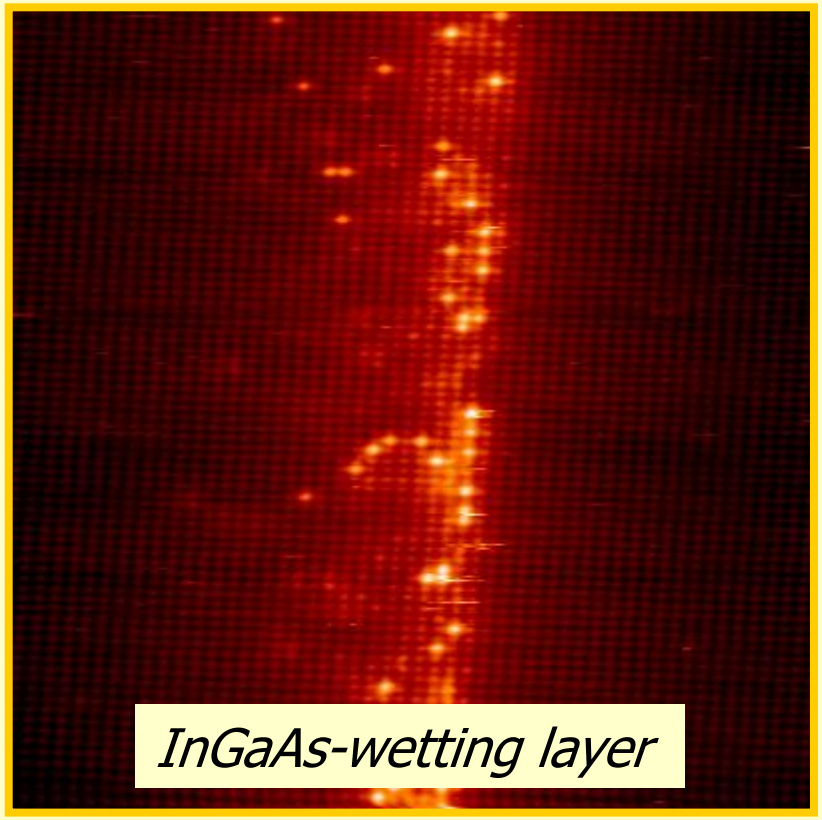
Two Si impurities in GaAs



UHV (10^{-11} torr)

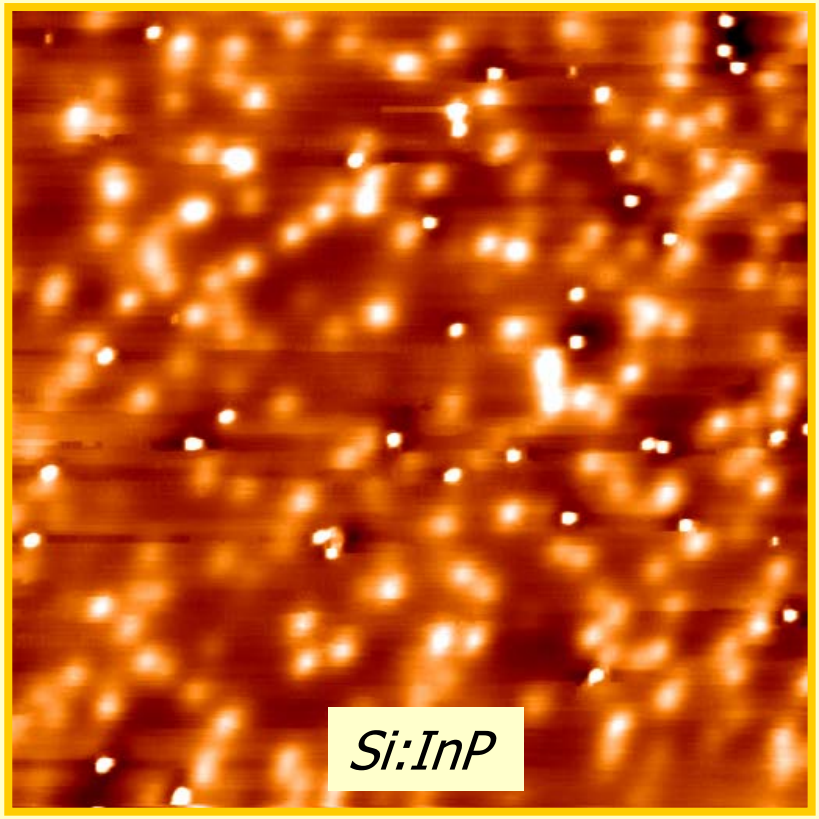
Impurity Imaging

Iso-electronic impurities



*30 nm * 30 nm*

Charged impurities

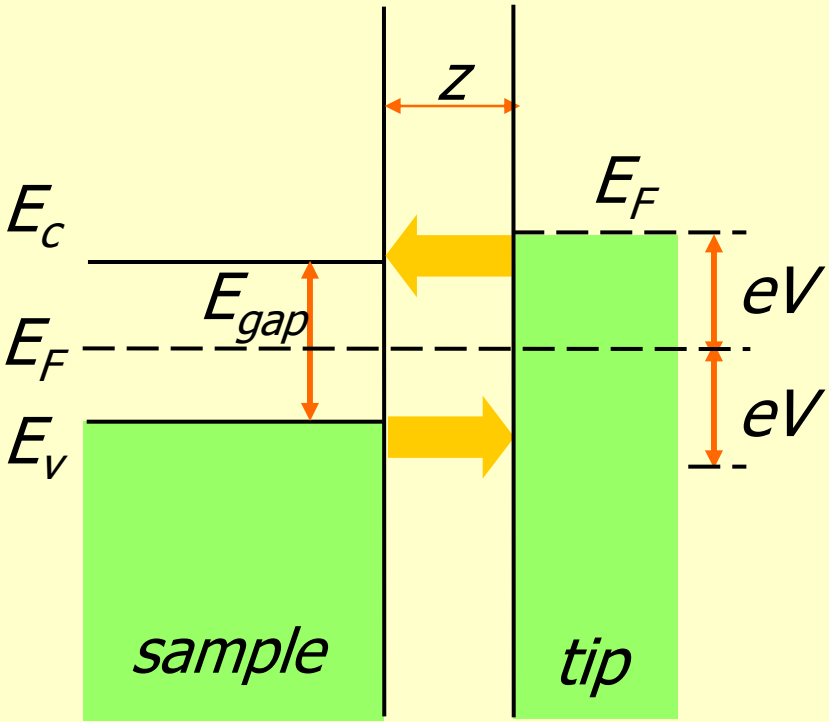


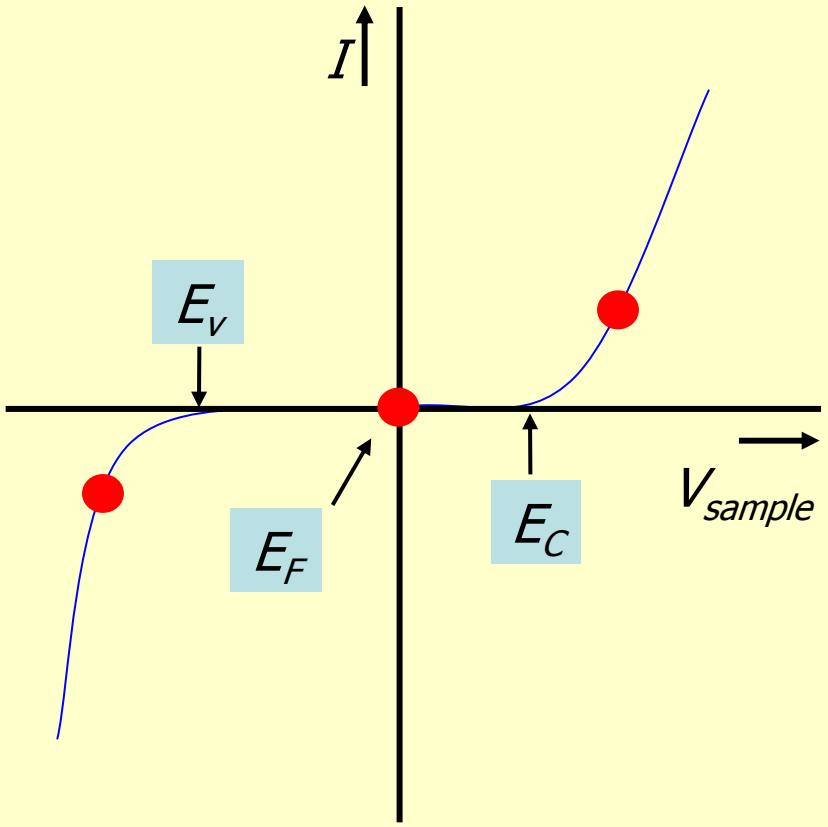
*100 nm * 100 nm*

Counting demonstrated up to 40 %

sharp (surface Si-atoms)
diffuse (sub-surface Si-ions)

Scanning Tunneling Microscopy on Semiconductors

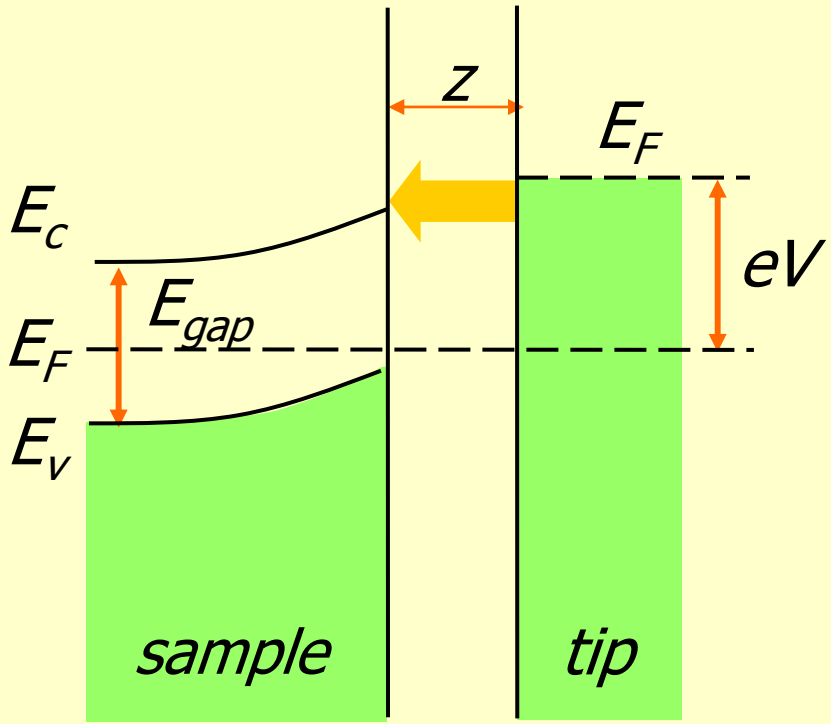




Scanning Tunneling Microscopy on Semiconductors

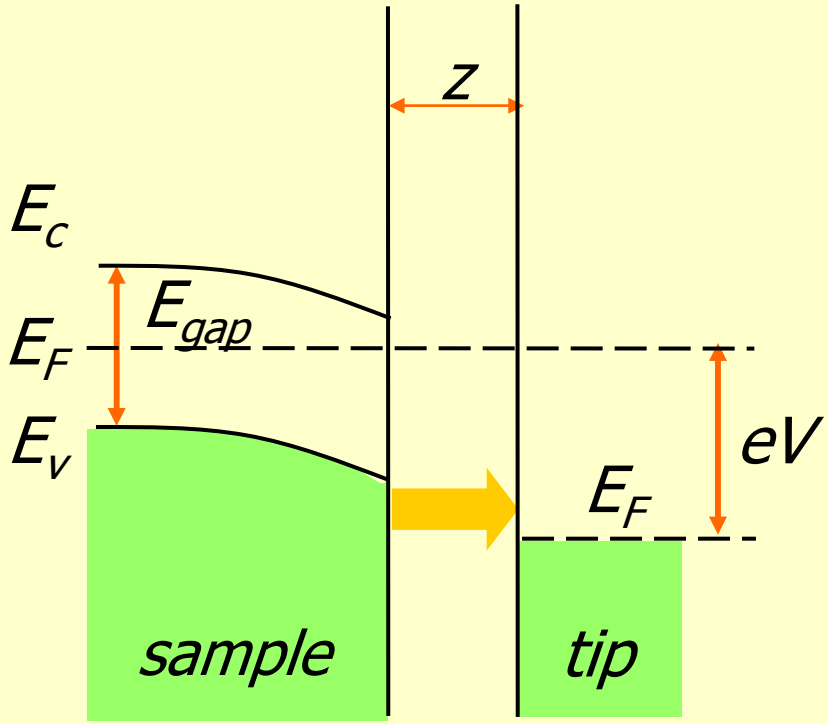
Positive *sample voltage*

(empty states)



Negative *sample voltage*

(filled states)

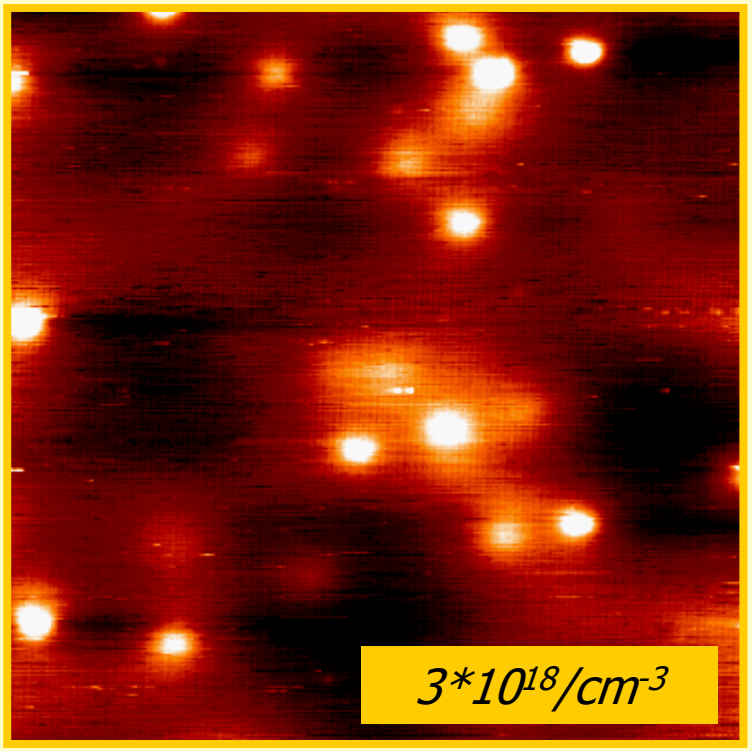


Depletion, accumulation, inversion

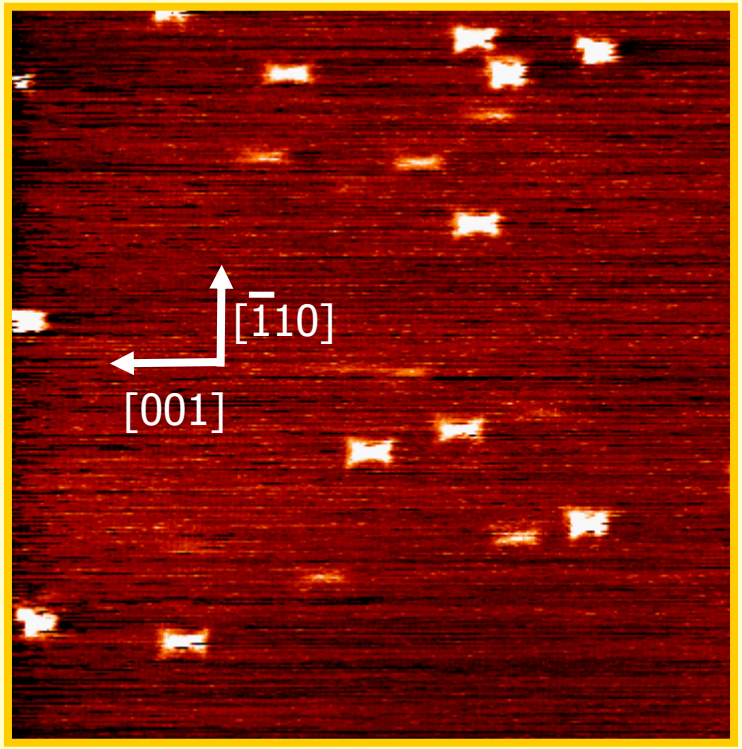
A^- and A^o Charge States of Mn

Ionized *Mn* A^-
(V=-1.1 V)

Neutral *Mn* A^o*:(ion + hole)*
(V=+1.1 V)



*70 nm * 70 nm*



*70 nm * 70 nm*

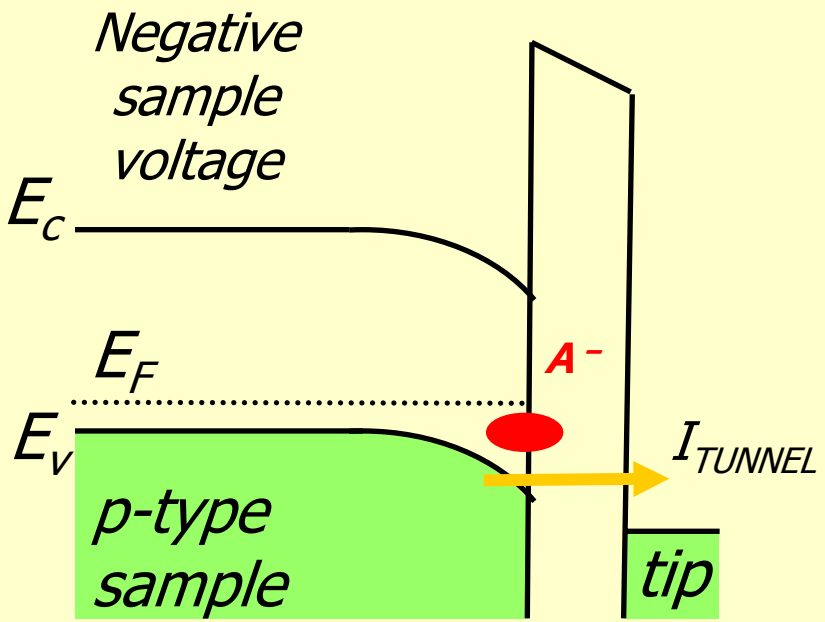
Grown by J. De Boeck et al., IMEC, Belgium

Same position is imaged at both voltages

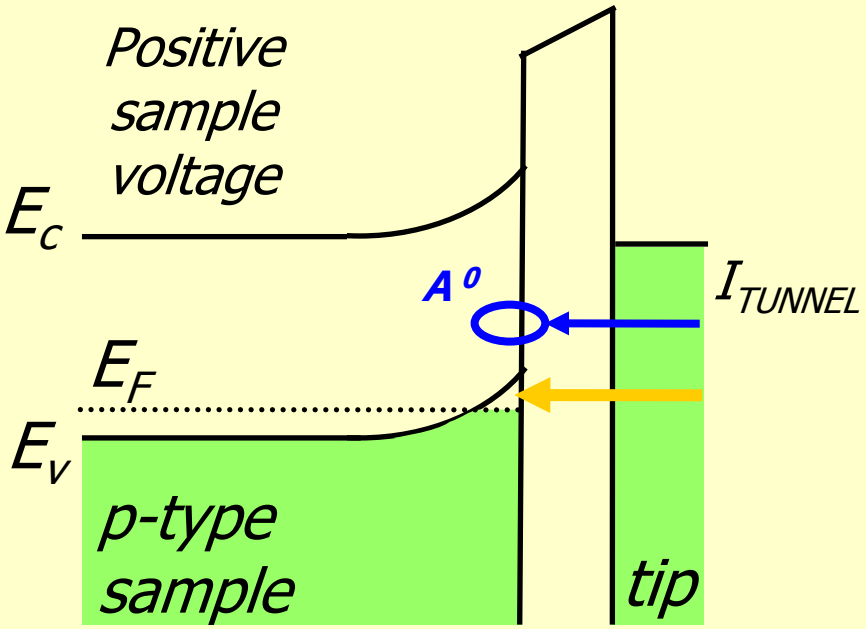
Contrast depends on depth of Mn-atom below cleaved surface

Manipulation of the Charge State by STM tip

Ionized *Mn acceptor*



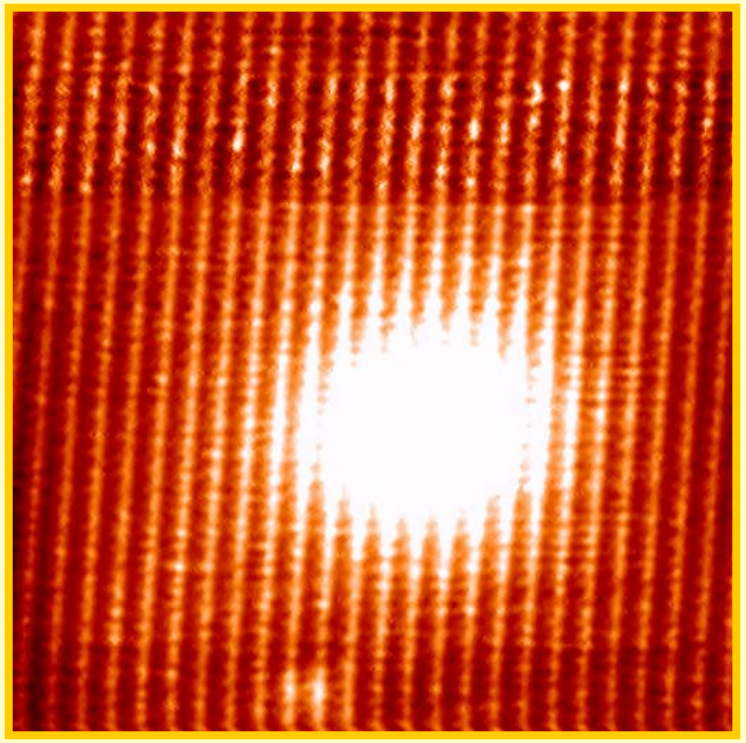
Neutral *Mn acceptor*



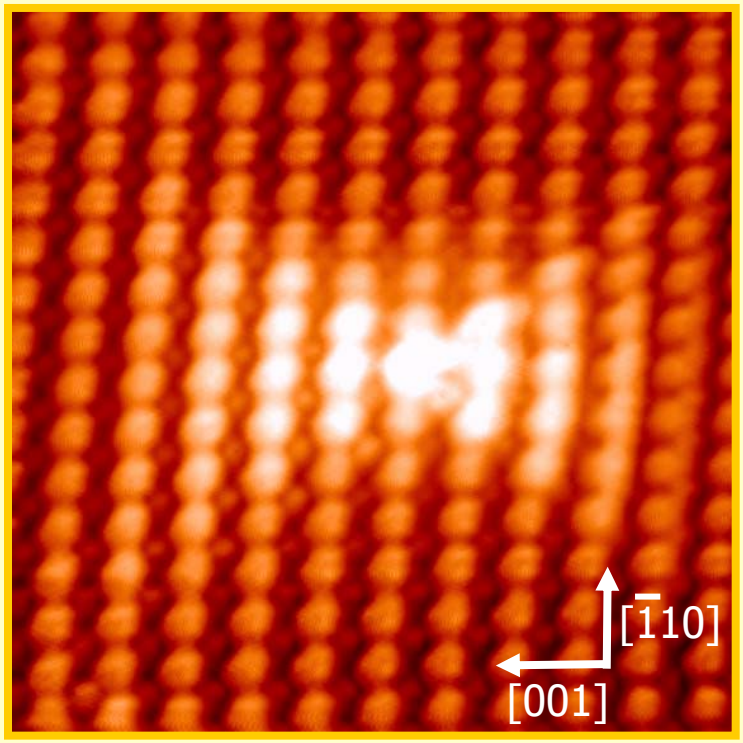
A^- and A^o Charge States of Mn

Ionized Mn A^-
(V=-0.9 V)

Neutral Mn A^o:(ion + hole)
(V=+0.7 V)



*14 nm * 14 nm*

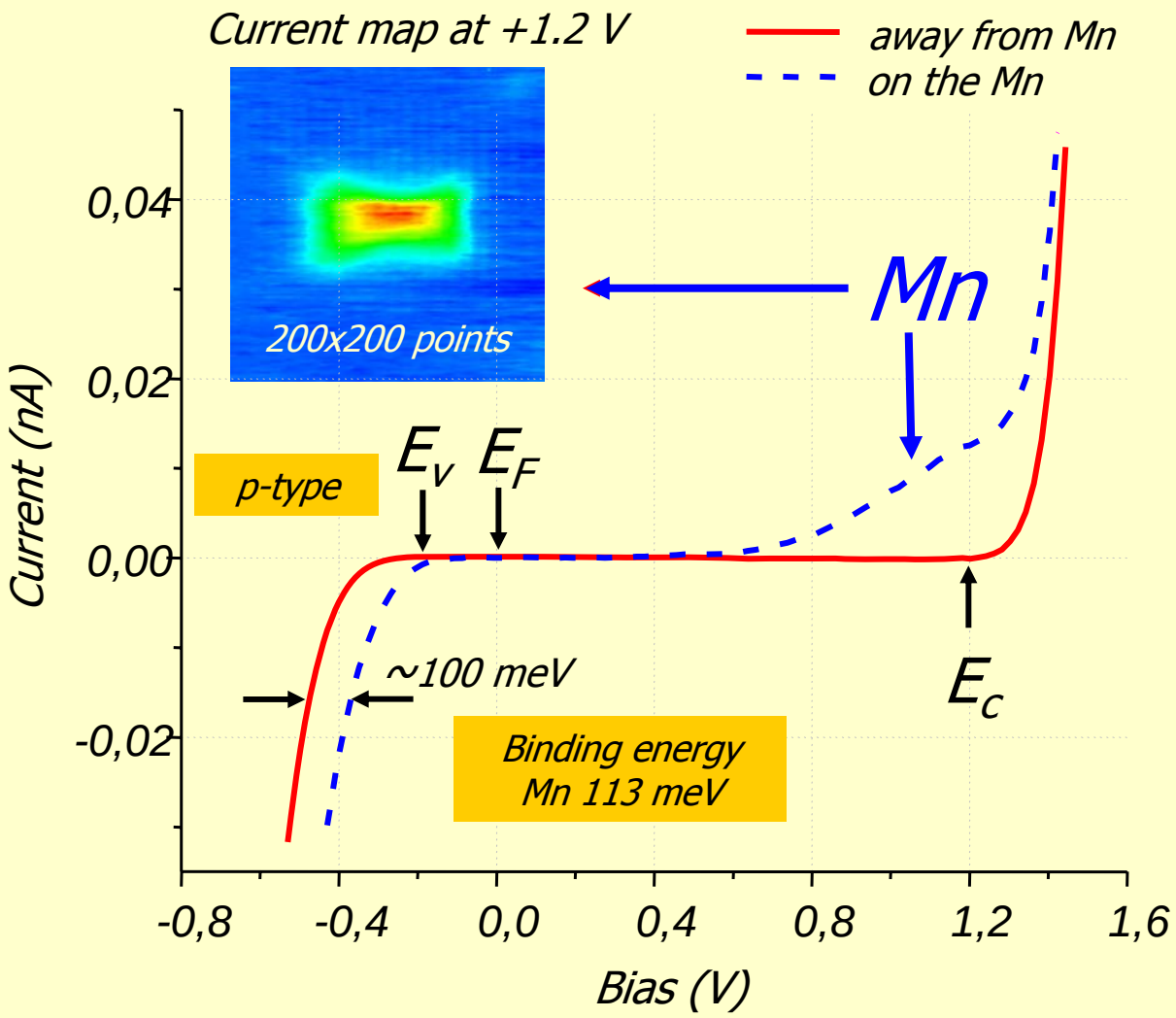


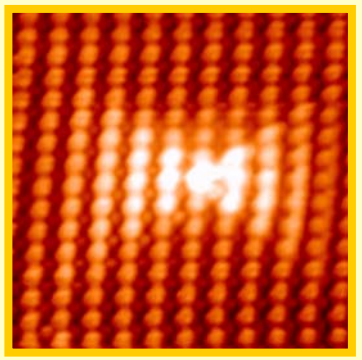
*5.6 nm * 5.6 nm*

Contrast is due to Coulomb field

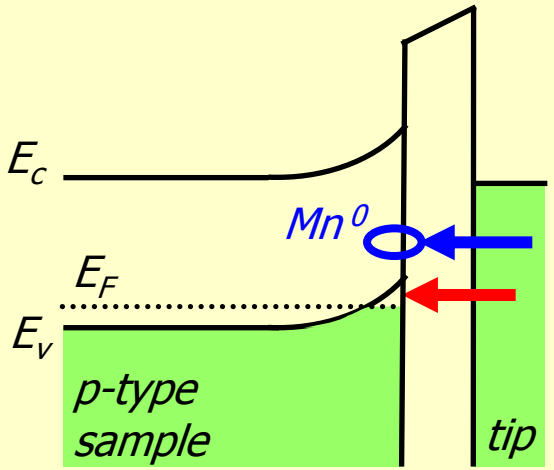
Tunneling to the bound hole
(Mn in ~ 3rd sublayer)

Spectroscopic Signature of Mn



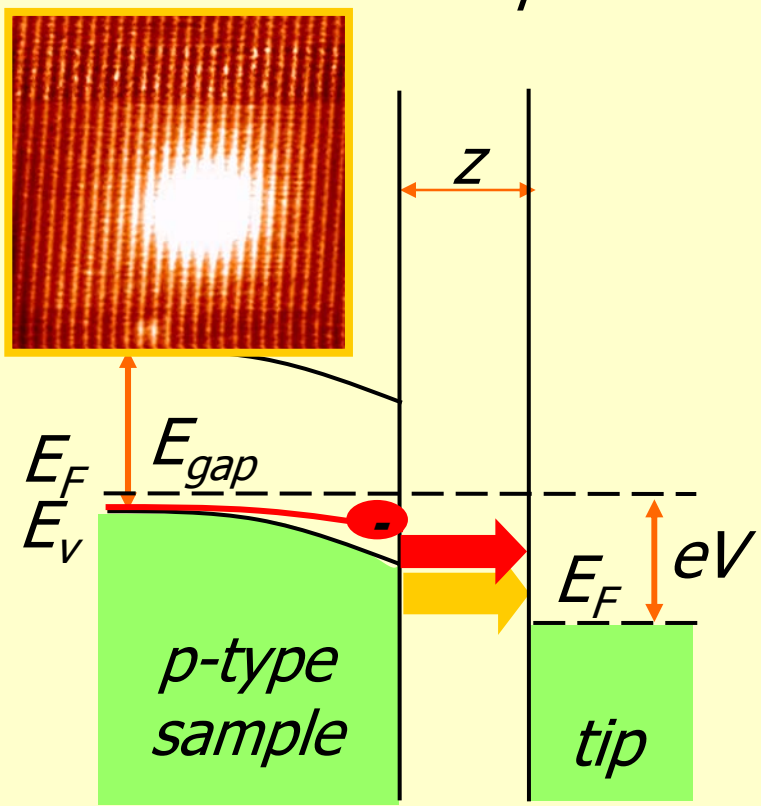


*200 * 200 I(V)-curves taken around impurity*



Contrast Mechanism

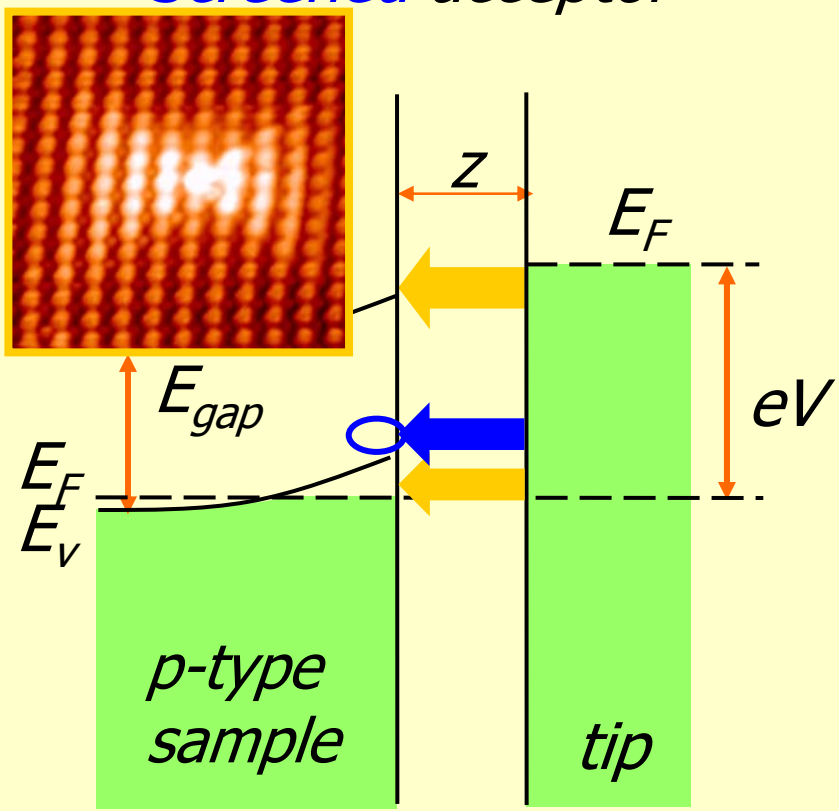
Ionized acceptor



Around charged acceptor bands bend upwards this increases current (height STM tip)

Bright feature

Screened acceptor

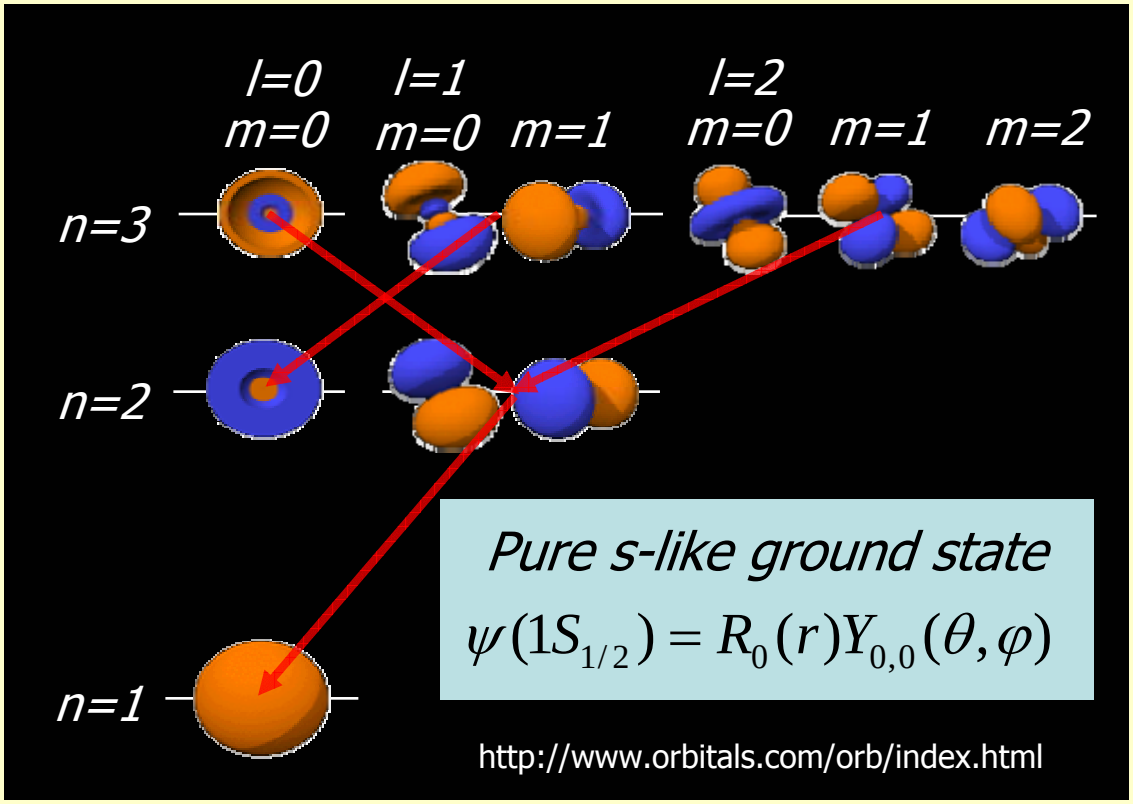


Around screened acceptor weak band bending. Due to impurity LDOS increase of current (height STM tip)

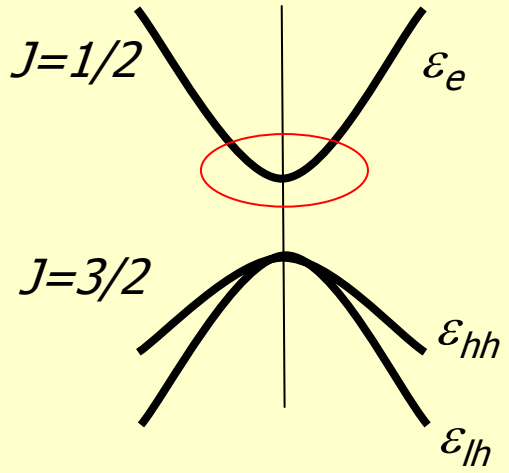
Bright feature

Modeling of Impurity States in Semiconductors

Effective Mass Donor

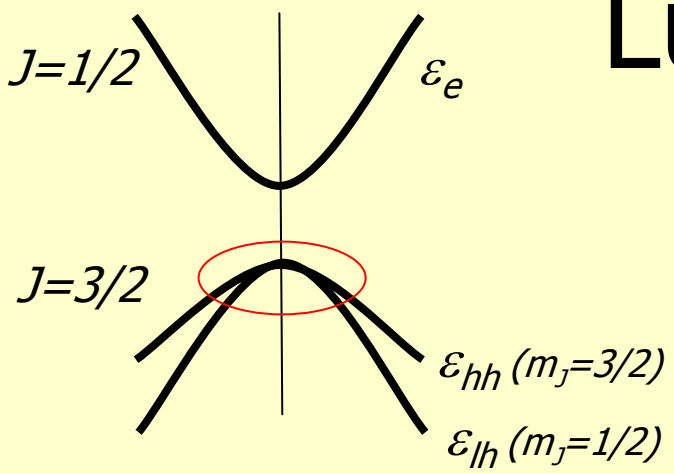


$$\varepsilon_e = \frac{\hbar^2}{2m^*}\left(k_x^2 + k_y^2 + k_z^2\right)$$



$$\frac{\hbar^2 k^2}{2m_e^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi_{n,l,m} + \frac{1}{\varepsilon_o \varepsilon_r r}\psi_{n,l,m} = \varepsilon_{n,l,m}\psi_{n,l,m}$$

Luttinger Hamiltonian



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

Luttinger Hamiltonian

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

$$\psi_i = \begin{pmatrix} \varphi_1 \cdot \left|3/2,+3/2\right\rangle \\ \varphi_2 \cdot \left|3/2,+1/2\right\rangle \\ \varphi_3 \cdot \left|3/2,-1/2\right\rangle \\ \varphi_4 \cdot \left|3/2,-3/2\right\rangle \end{pmatrix}$$

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

Spin-orbit coupling mixes the light and heavy hole bands in confined states

$\gamma_2 = \gamma_3$ isotropic dispersion

Effective Mass Acceptor

$$H_{Lut}\psi_{n,l,m} + \frac{1}{\varepsilon_o \varepsilon_r r}\psi_{n,l,m} = \varepsilon_{n,l,m}\psi_{n,l,m}$$

Isotropic dispersion

Ground state components

$$\psi_{3/2}^{3/2} = R_0 \begin{pmatrix} Y_{0,0} \\ 0 \\ 0 \\ 0 \end{pmatrix} + \beta \cdot R_2 \begin{pmatrix} \sqrt{2}Y_{2,0} \\ -2Y_{2,1} \\ 2Y_{2,2} \\ 0 \end{pmatrix} \qquad \psi_{1/2}^{3/2} = R_0 \begin{pmatrix} 0 \\ Y_{0,0} \\ 0 \\ 0 \end{pmatrix} + \beta \cdot R_2 \begin{pmatrix} 2Y_{2,-1} \\ -\sqrt{2}Y_{2,0} \\ 0 \\ 2Y_{2,2} \end{pmatrix}$$

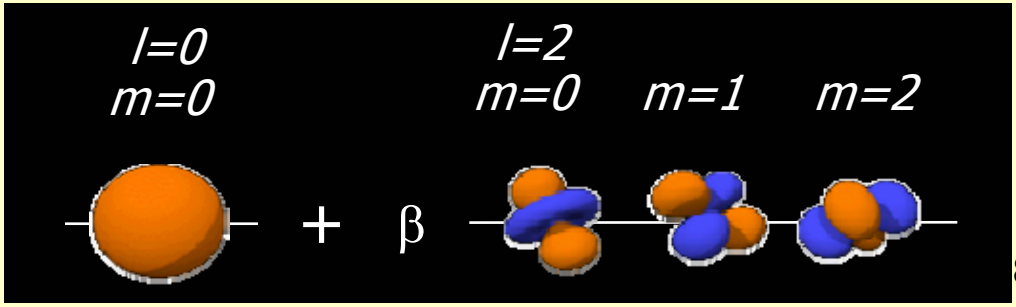
$Y_{l,m}$ spherical harmonics

R_l radial distribution

and their Kramers conjugates $\psi_{-3/2}^{3/2}$ *and* $\psi_{-1/2}^{3/2}$

Bir, Pikus in "Symmetry and strain-induced effects in semiconductors"

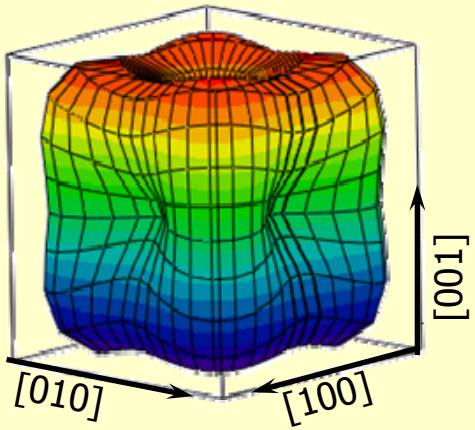
the ground state has a mixed s + d character



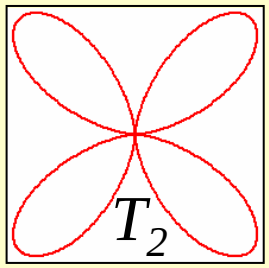
Effective Mass Acceptor

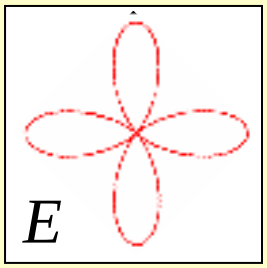
$$H_{Lut}\psi_{n,l,m} + \frac{1}{\varepsilon_o \varepsilon_r r}\psi_{n,l,m} = \varepsilon_{n,l,m}\psi_{n,l,m}$$

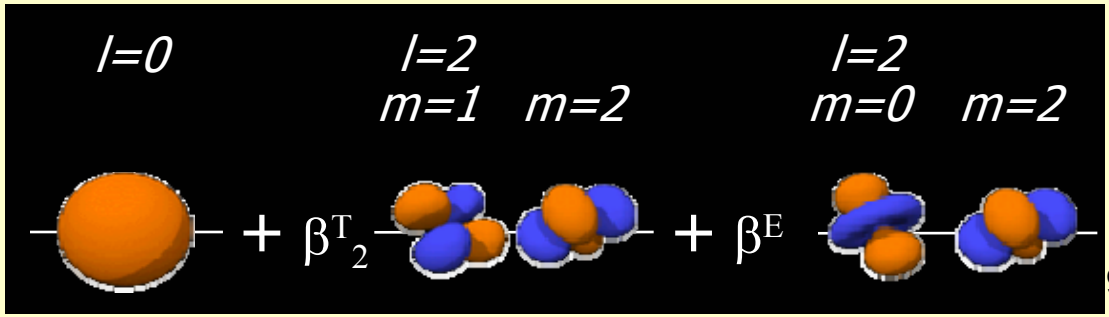
$$\psi_{3/2}^{3/2} = R_0 \begin{pmatrix} Y_{0,0} \\ 0 \\ 0 \\ 0 \end{pmatrix} + \beta^{T_2} \cdot R_2 \begin{pmatrix} 0 \\ 2Y_{2,1} \\ Y_{2,2} - Y_{2,-2} \\ 0 \end{pmatrix} + \beta^{E} \cdot R_2 \begin{pmatrix} \sqrt{2}Y_{2,0} \\ 0 \\ Y_{2,2} + Y_{2,-2} \\ 0 \end{pmatrix}$$



Cubic symmetry of crystal selects d-components





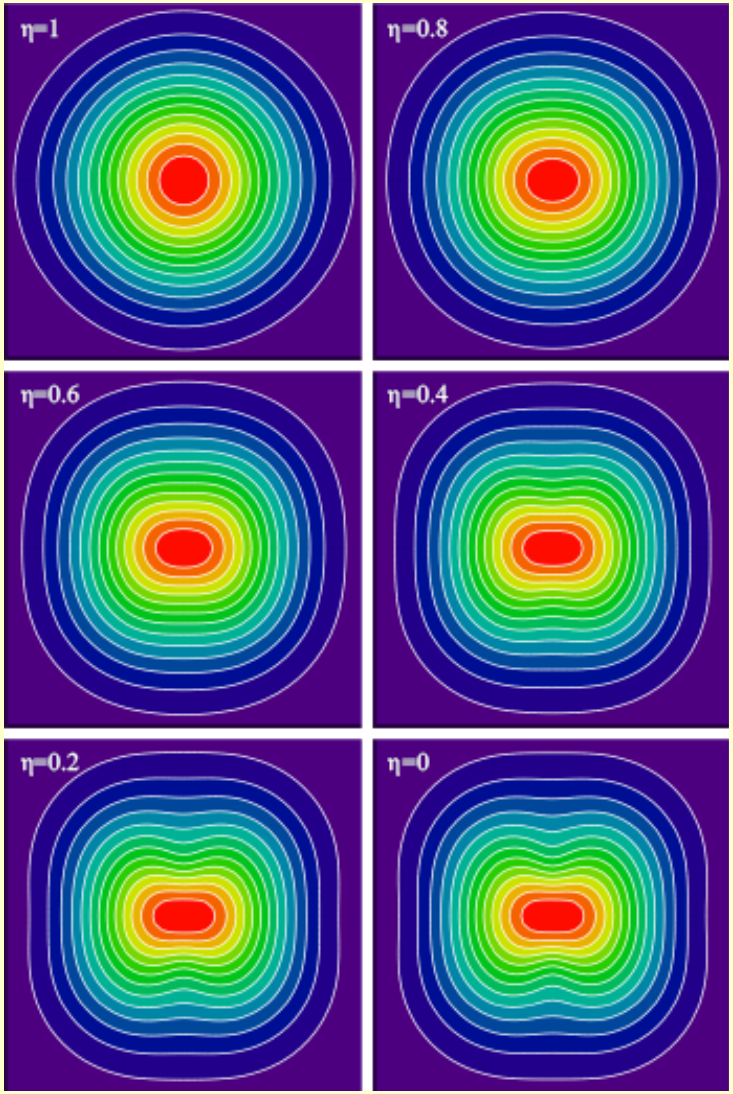


Effect of Crystal Anisotropy

η=1 corresponds with isotropic dispersion

η=0 corresponds with a pure T_2 symmetry

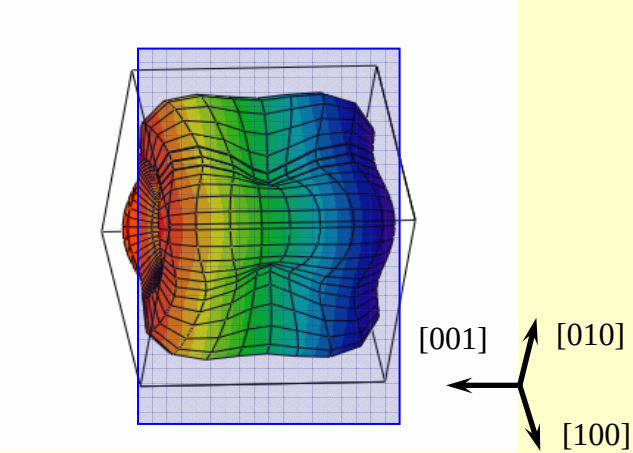
$$\eta = \frac{\beta_E}{\beta_{T_2}}$$



*8 nm * 8 nm*

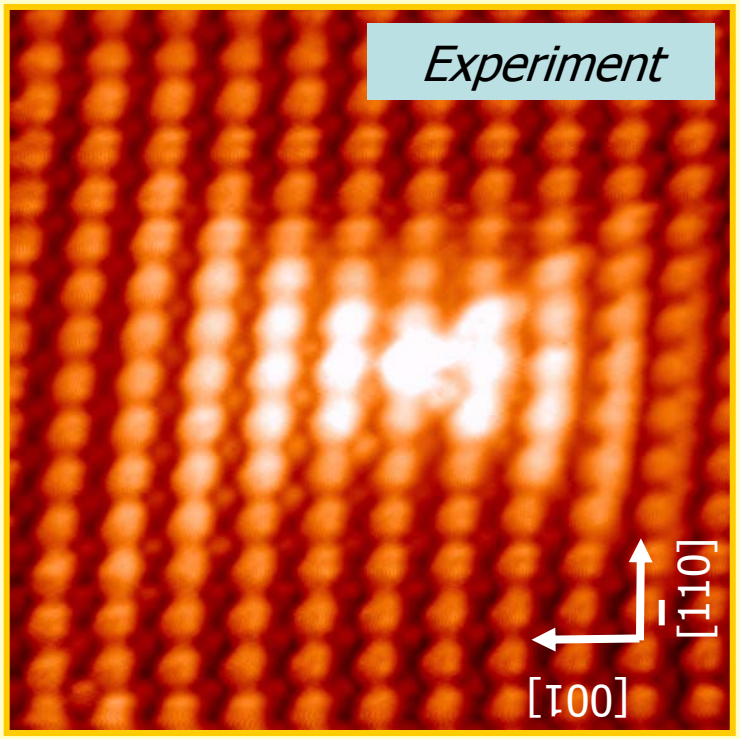
Cut at 6 monolayer's trough impurity state along a 110 plane

Effective mass model



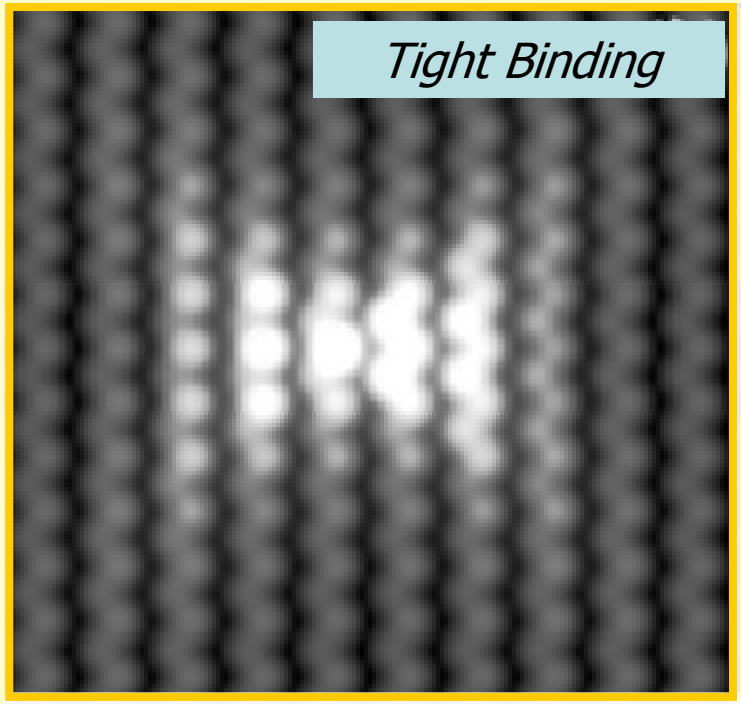
110 plane

Electronic Structure of Mn-acceptor



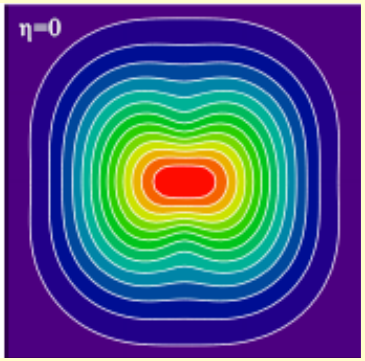
6 nm * 6 nm

Grown by J. De Boeck et al., IMEC, Belgium



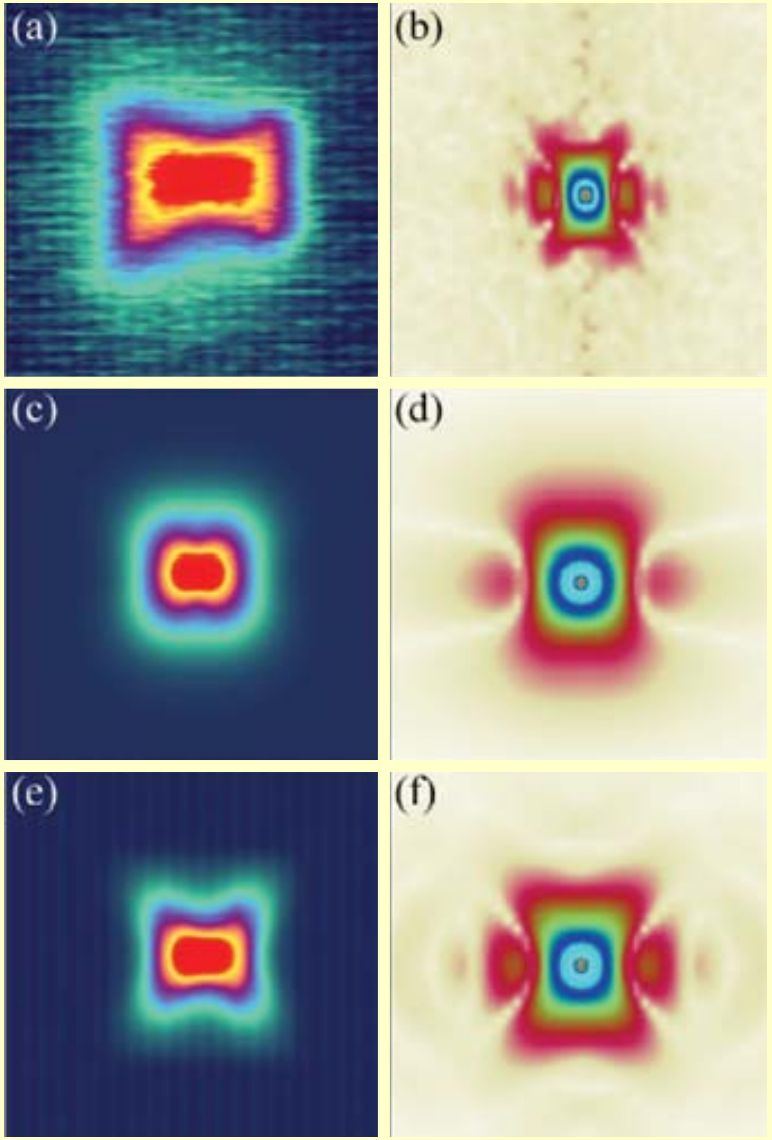
J.-M. Tang M. Flatté, Iowa, US

Effective mass model



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

Real Space *Fourier Space*



*12 nm *12 nm* *0.8 nm^{-1}* 0.8 nm^{-1}*

Experiment

Mn in ~ 4th sublayer

Effective mass model

$$\eta = \beta^{E} / \beta^{T_2} = 0$$

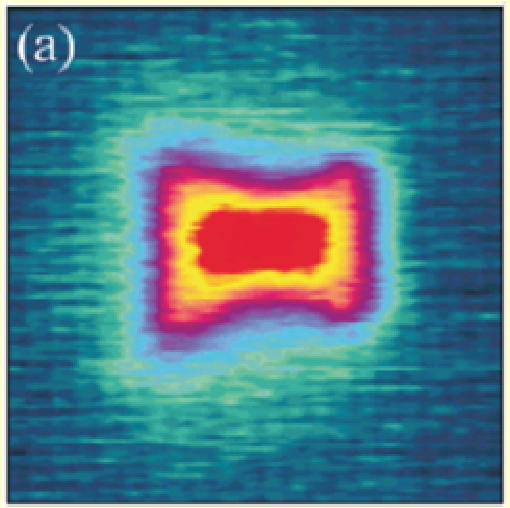
Tight-binding model
(M. Flatté, University of Iowa)

$$\eta = \beta^{E} / \beta^{T_2} \approx 0$$

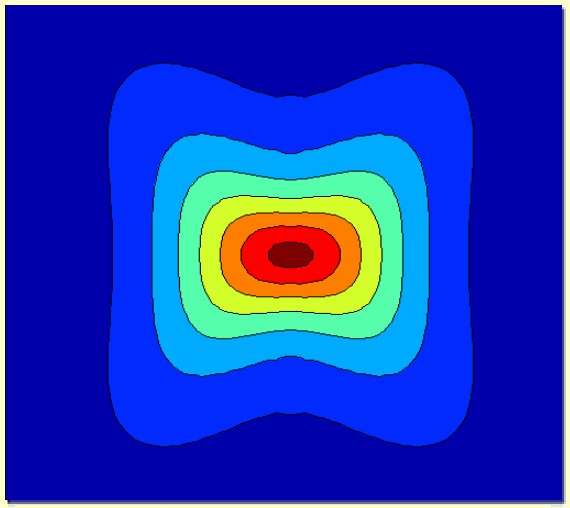
*Yakunin et al. PRL **92**, 216806 (2004)*

Improved Effective Mass Model

Experiment



Effective mass model



Inclusion of anisotropy ($\gamma_2 \neq \gamma_3$) in the dispersion

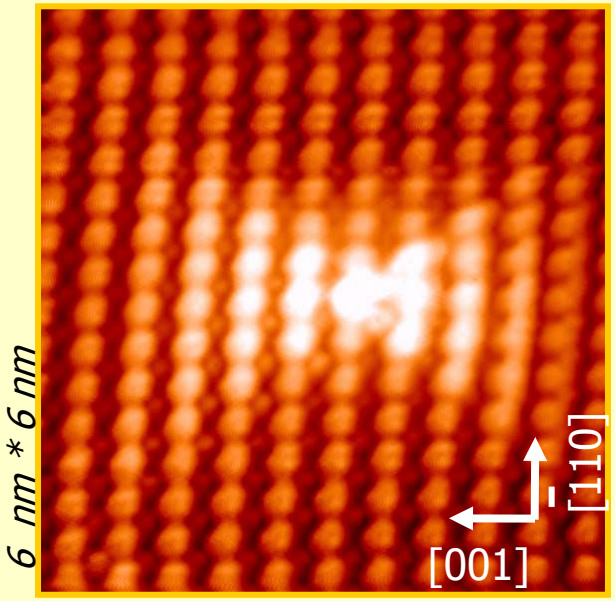
A. Monakhov & N. Averkiev, Ioffe Institute

Symmetry Breaking

by crystal symmetry

Broken Symmetry

Mn:GaAs

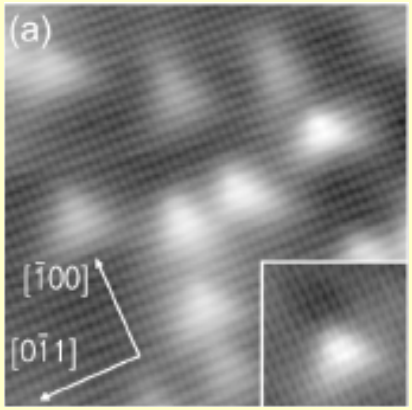


*Yakunin et al. PRL **92**, 216806 (2004)*

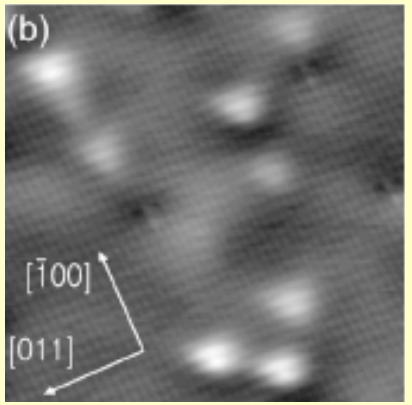
Bulk or surface symmetry??

Zn:GaAs

110-surface



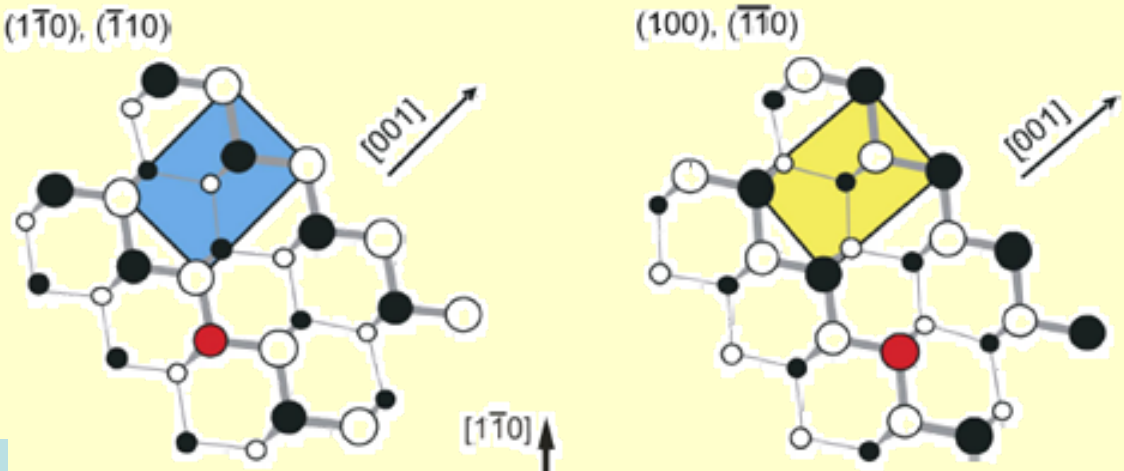
1-10-surface



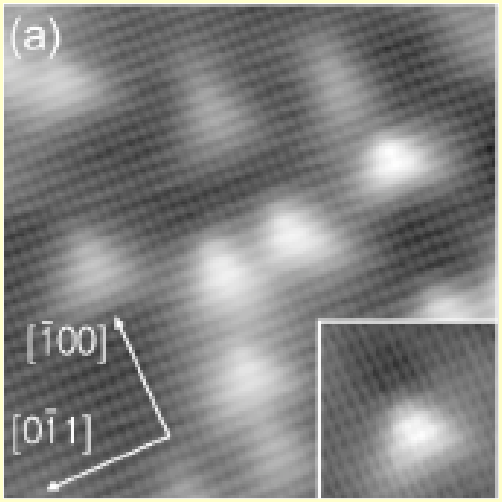
*Mathieu et al. PRL **94**, 026407 (2005)*

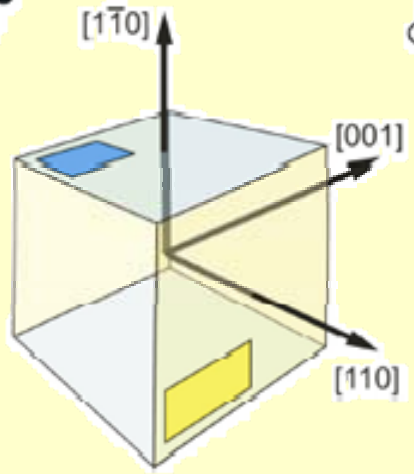
Inversion Asymmetry

Figure: S. Loth, Goettingen

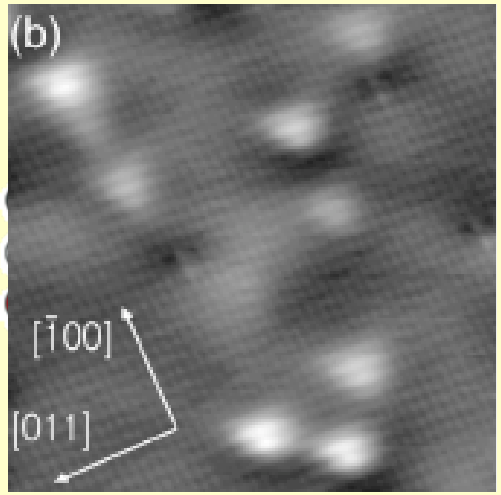


110-surface



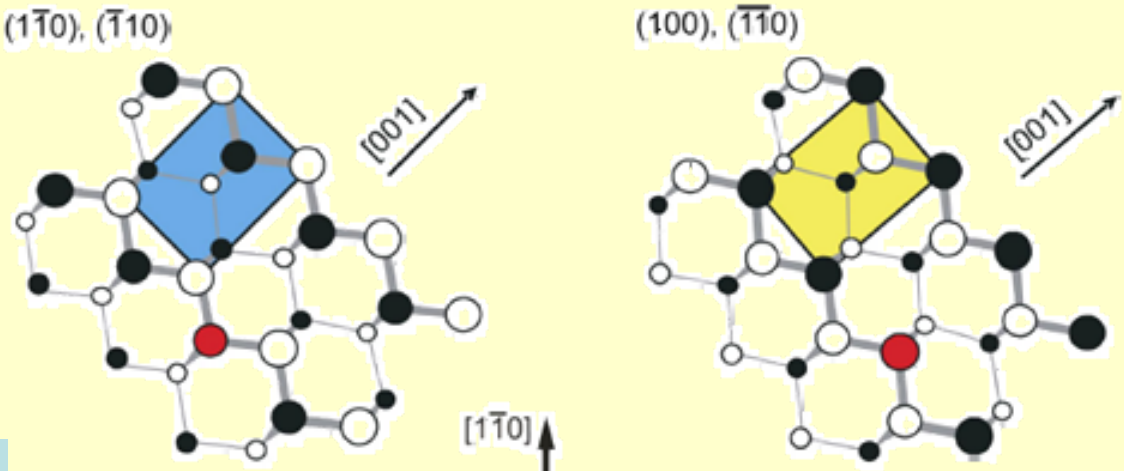


1-10-surface

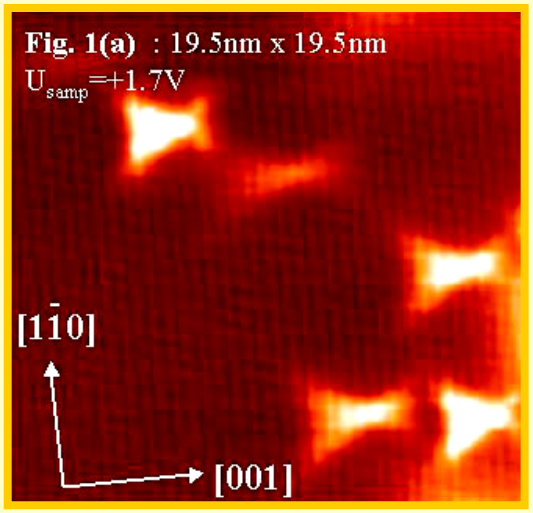


Mathieu et al.
*PRL **94**, 026407 (2005)*

Inversion Asymmetry



110-surface



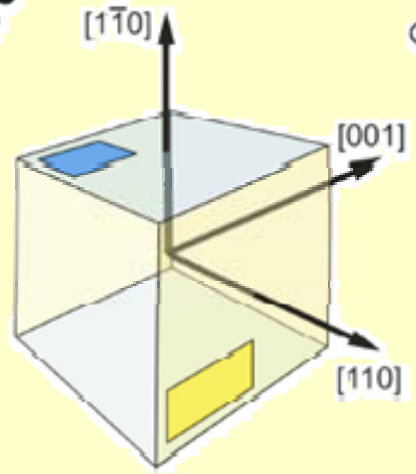
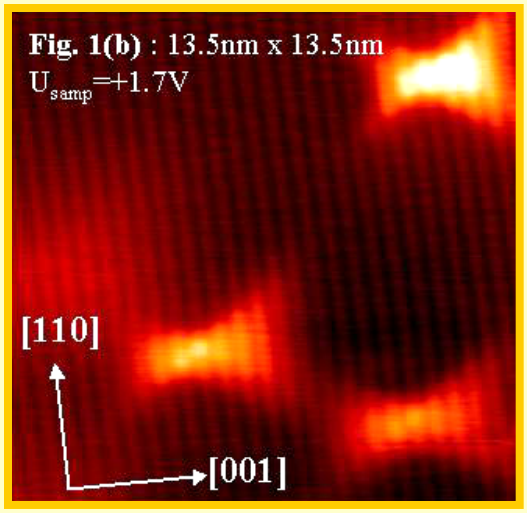


Figure: S. Loth, Goettingen

1-10-surface



Symmetry Breaking

by strain

Stacked Quantum Dots

*55 nm * 55 nm*

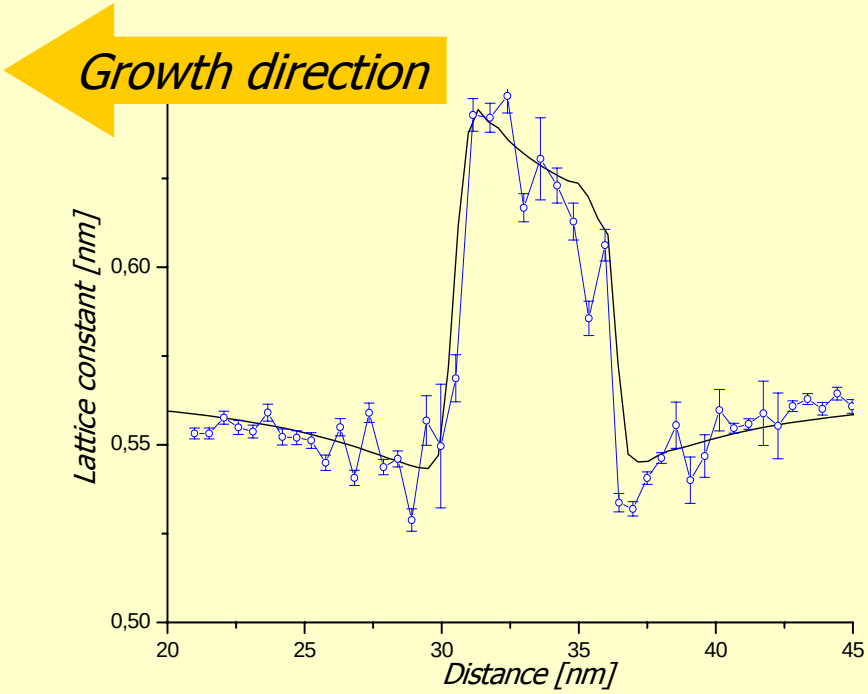
Grown by M. Hopkinson, Sheffield (UK)

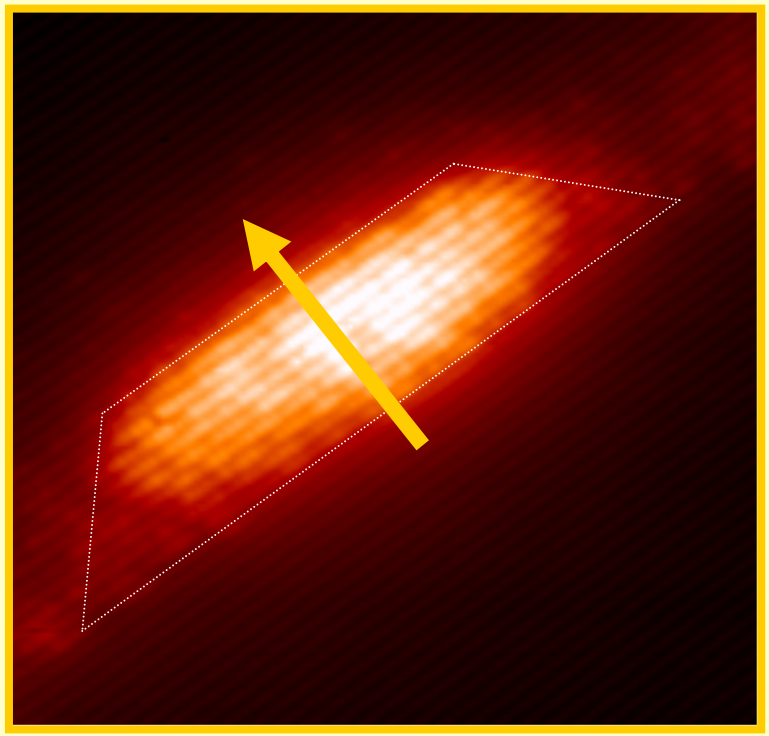
current image

*Bruls et al. APL **82**, 3758 (2003)*

Lattice Constant Profile

InAs/GaAs dot

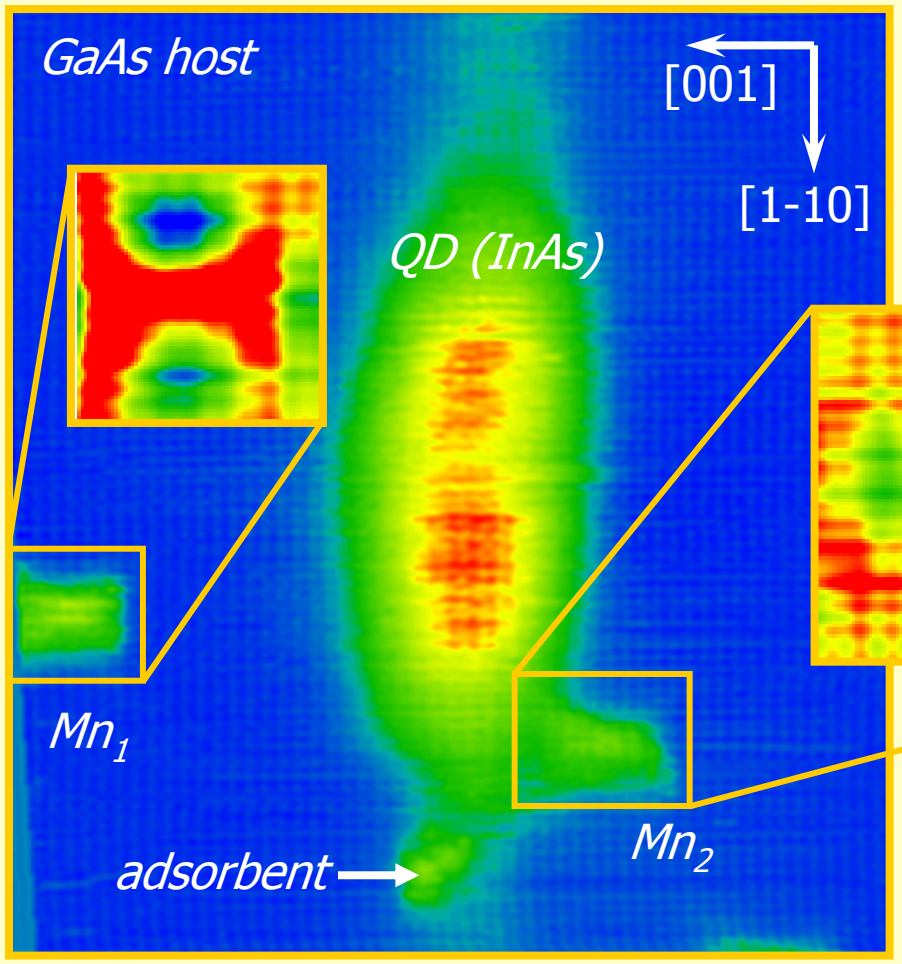




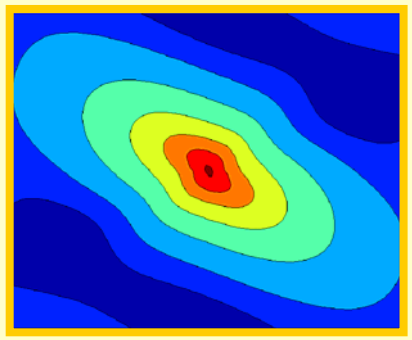
*22 nm * 22 nm*

Grown by K. Pierz, PTB-Braunschweig, Germany

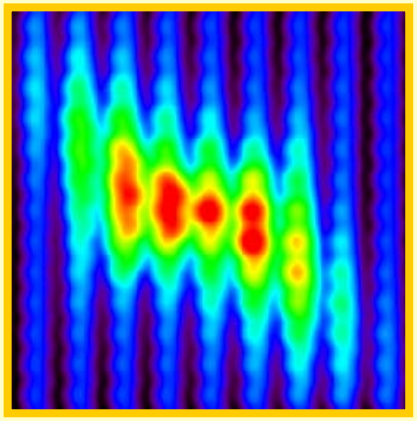
Strained Mn impurity



Fourier filtered experimental image



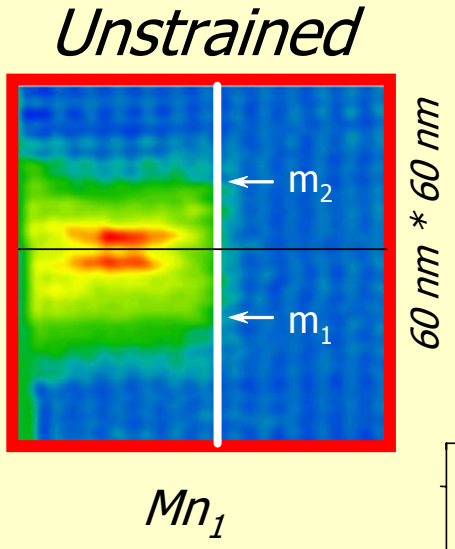
Effective mass

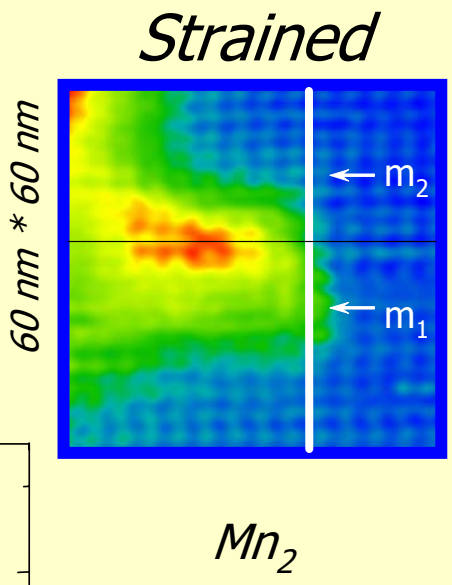


TBM

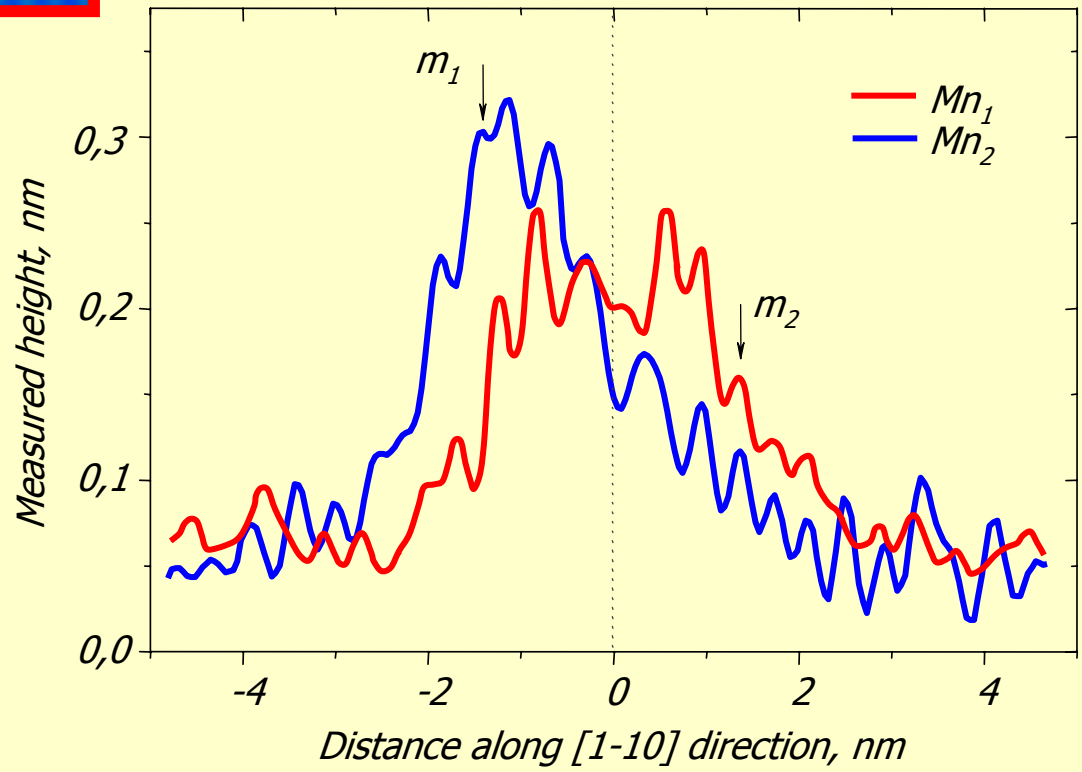
Grown by J. De Boeck et al., IMEC, Belgium

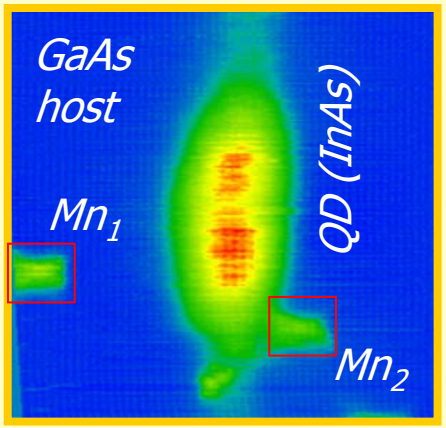
Strained Mn impurity



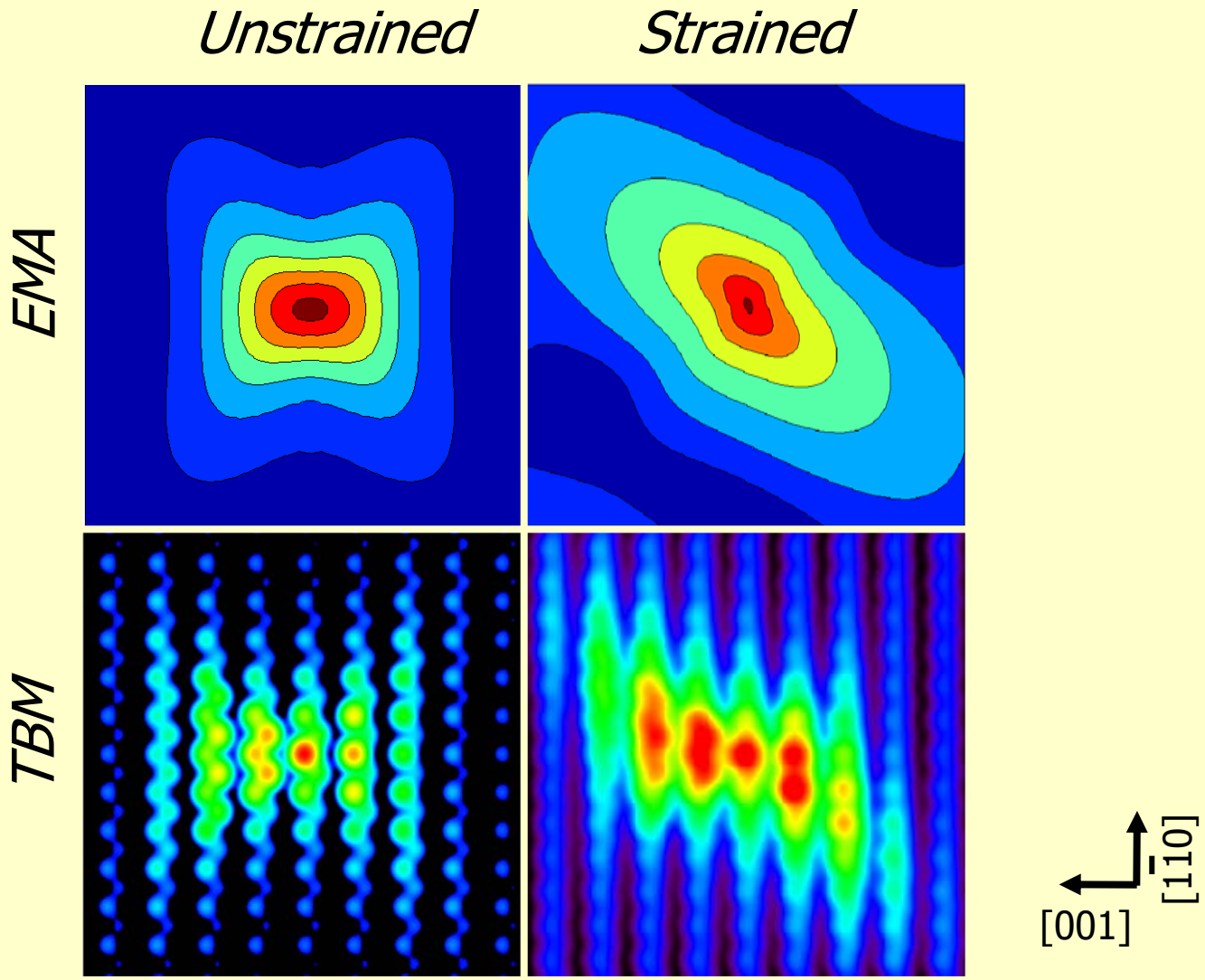


[001]
[1-10]





Strained Mn impurity

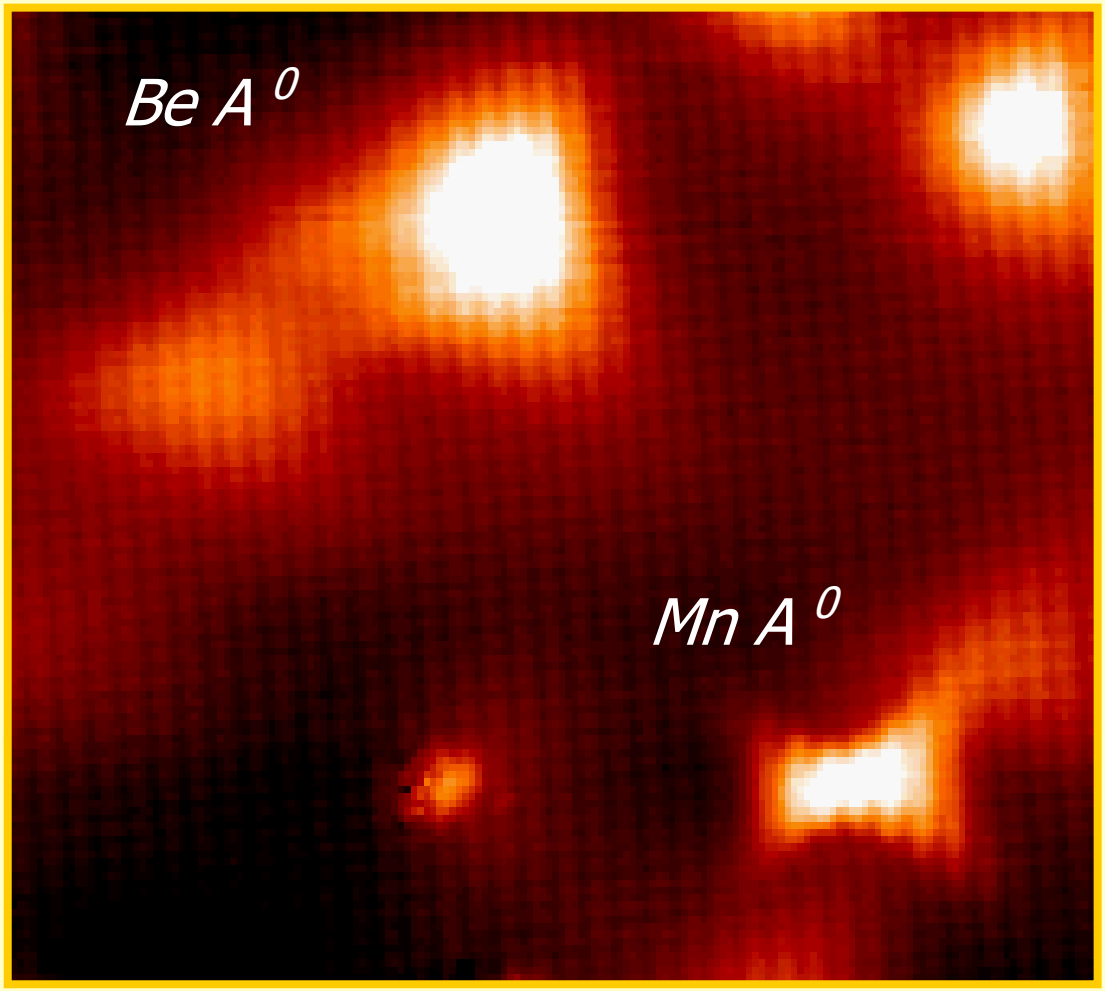


Symmetry Breaking

Shallow Impurities

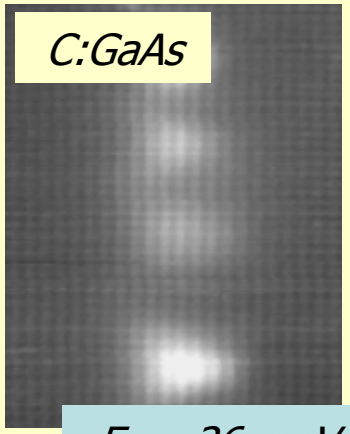
Broken Symmetry Shallow Impurities

Co-doped GaAs:Be,Mn



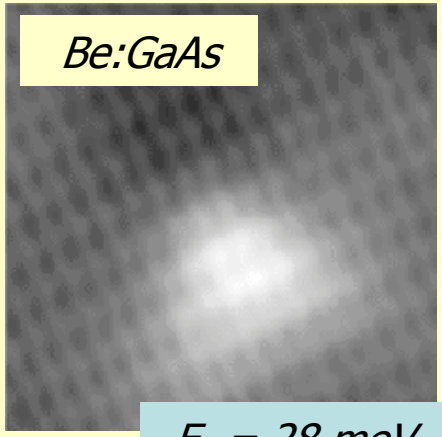
*30 nm * 30 nm*

Shallow & Deep Acceptor states



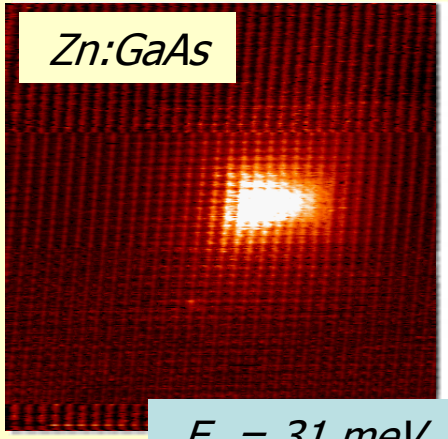
E_B = 26 meV

Reusch et al.
Univ. Of Gottingen



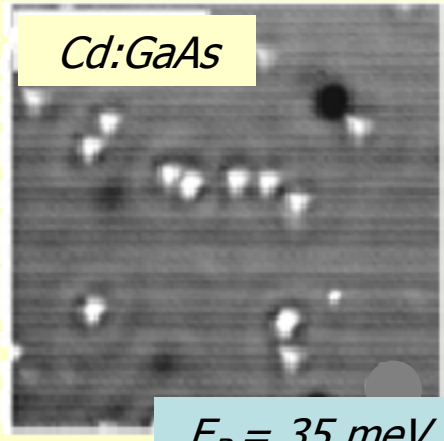
E_B = 28 meV

Mahieu et al.
PRL **94**, 026407 (2005)



E_B = 31 meV

Zheng et al.
APL **64**, 1836 (1994)



E_B = 35 meV

van der Wielen et al.
PRB **63**, 125336 (2001)

Shallow

Mn
113 meV

Co
150 meV

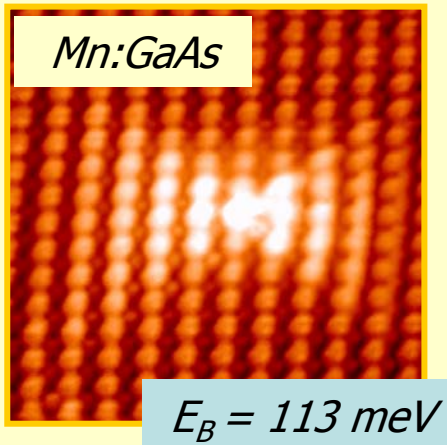
Cd
35 meV

Zn
30 meV

Be
28 meV

C
26 meV

Valence band

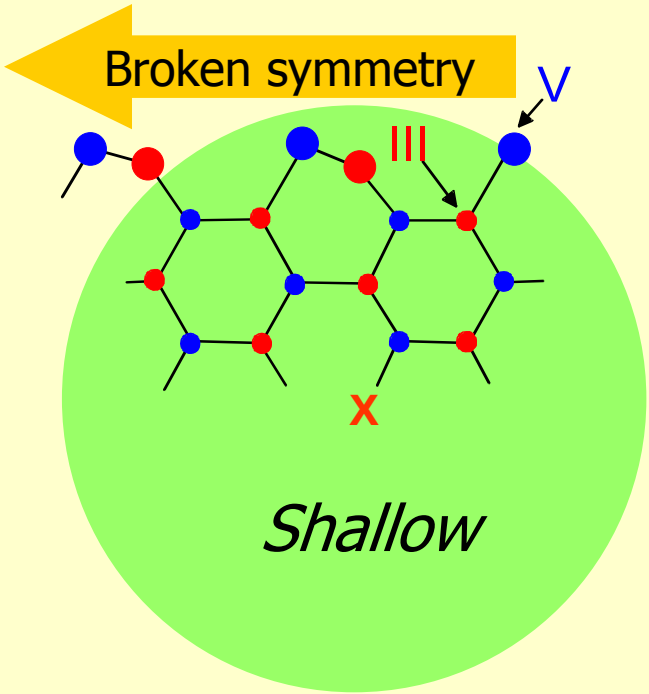


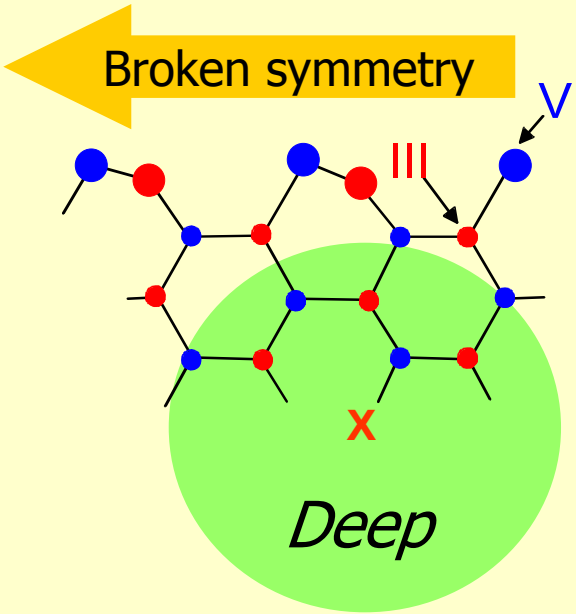
E_B = 113 meV

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

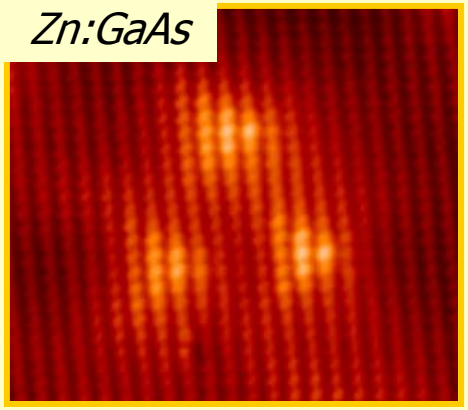
Deep

Interaction with Surface





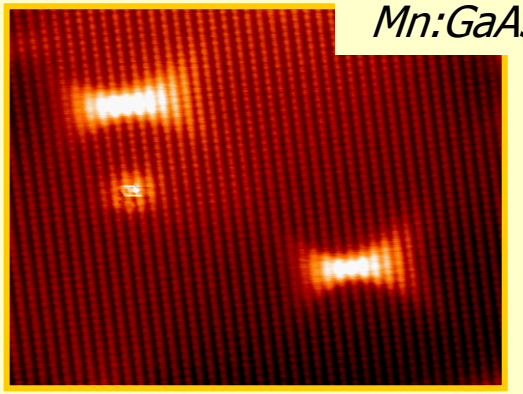
Zn:GaAs



Effective localization radius of a neutral acceptor

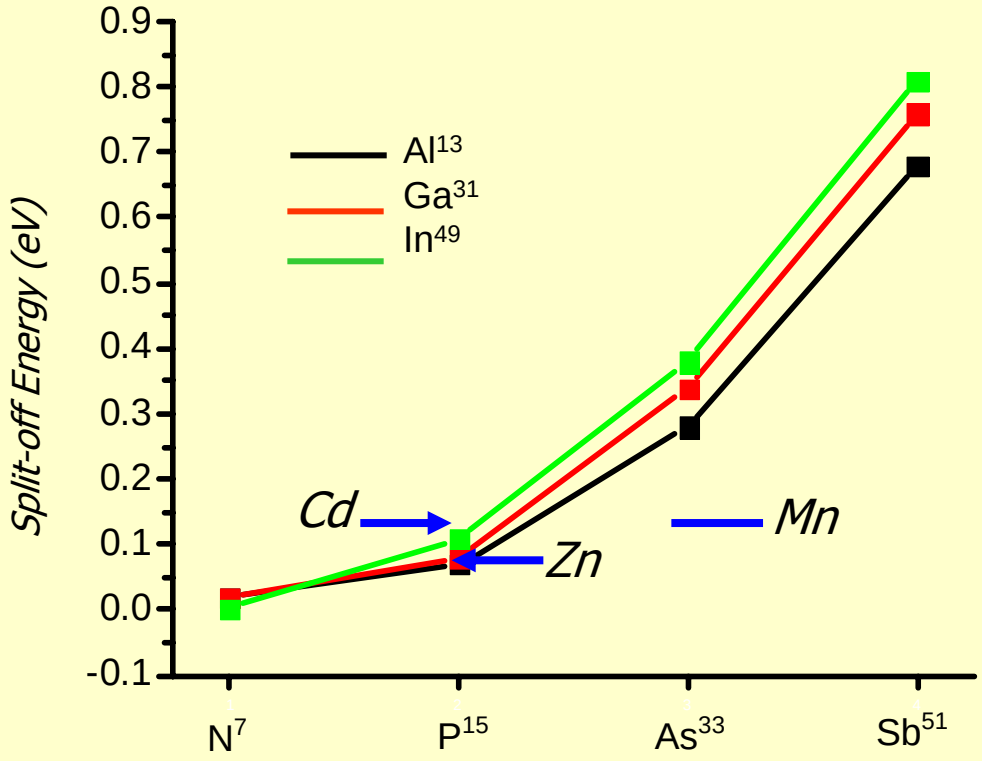
$$a_0 = \sqrt{\frac{\hbar^2}{2m^* E_b}}$$

Mn:GaAs

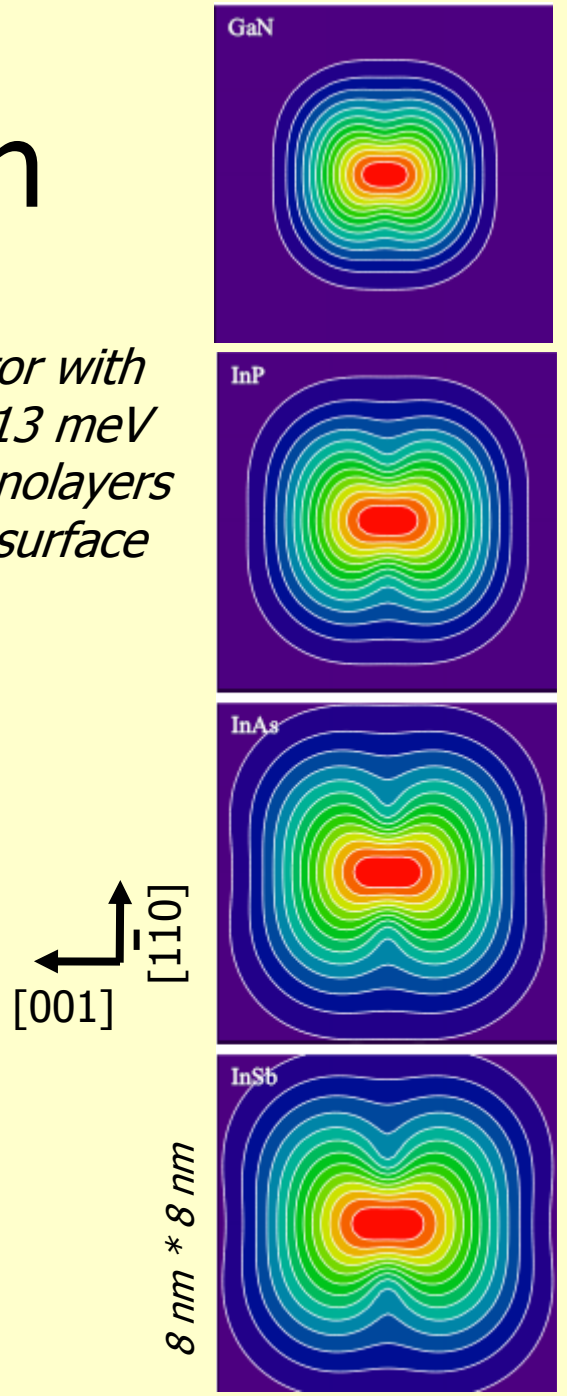


Spin-orbit Interaction

Spin-orbit Interaction

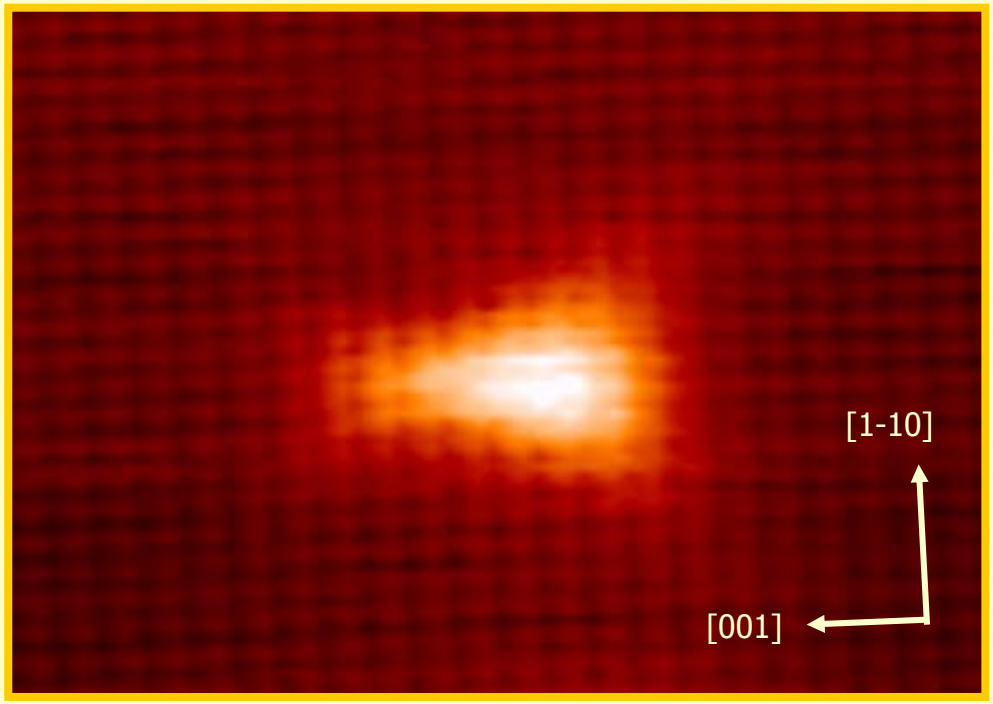


Acceptor with E_b = 113 meV at 6 monolayers below surface



Spatial Structure of Zn in GaP(110)

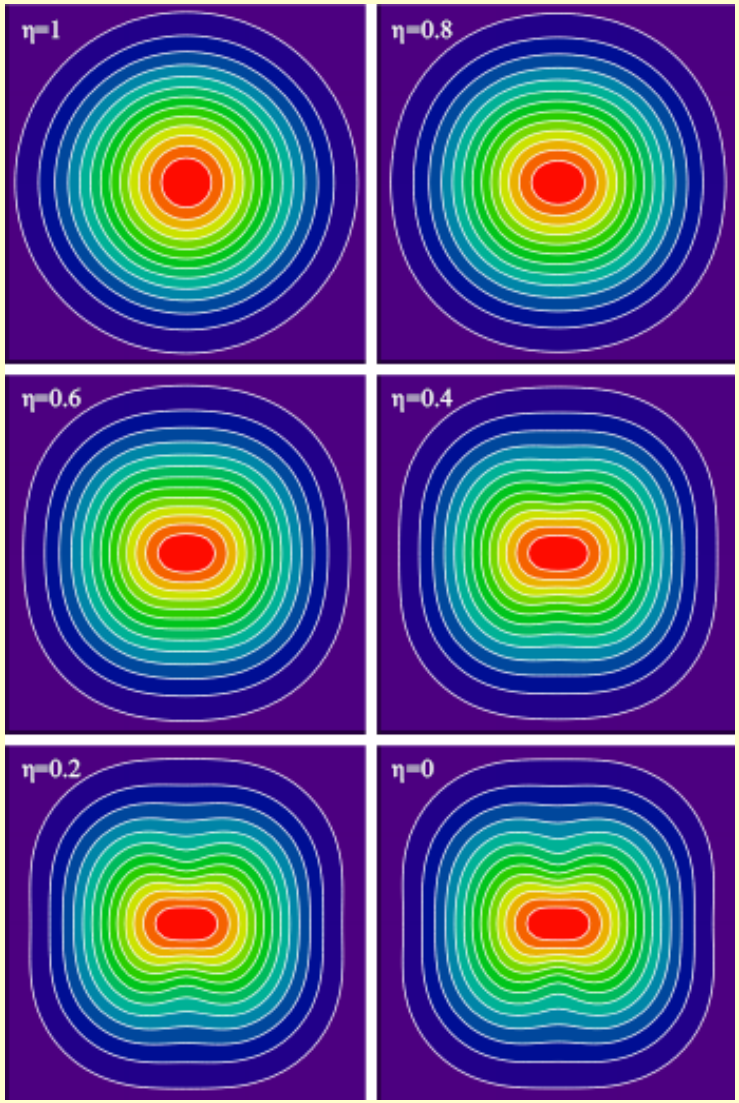
Bulk GaP intentionally doped with Zn (~2x10^{18}cm^{-3})

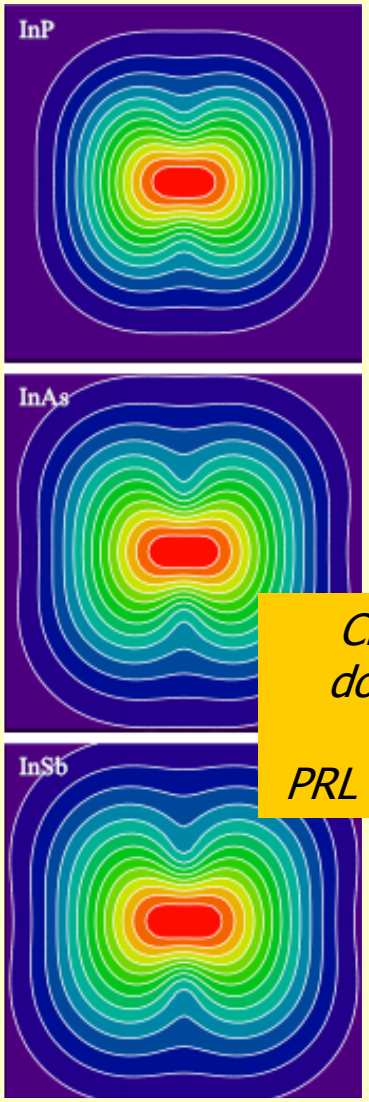


Anisotropy & Spin-orbit Interaction

η=1 corresponds with isotropic dispersion

η=0 corresponds with a pure T_2 symmetry





Acceptor with E_b = 113 meV

at 6 monolayers below surface

*Crystal anisotropy dominates see also Yakunin et al. PRL **92**, 216806 (2004)*

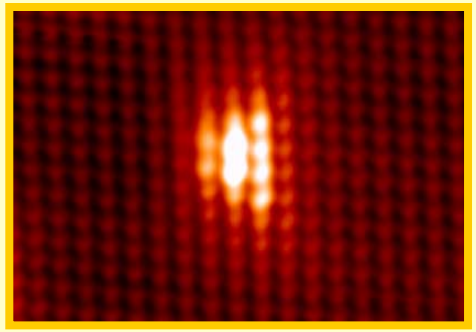
*8 nm * 8 nm*

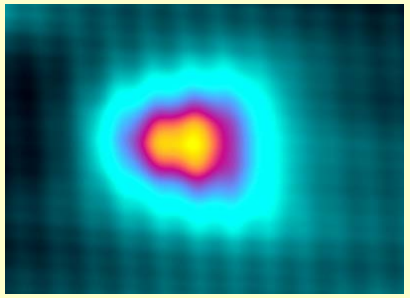
Missing link

Topography image

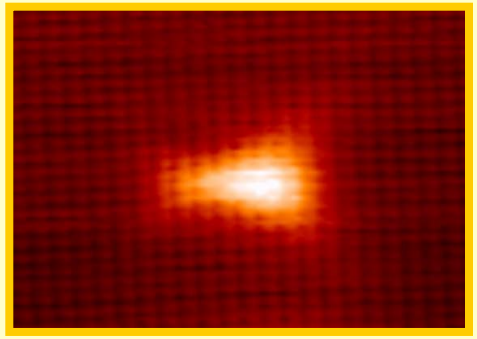
Fourier filtered image

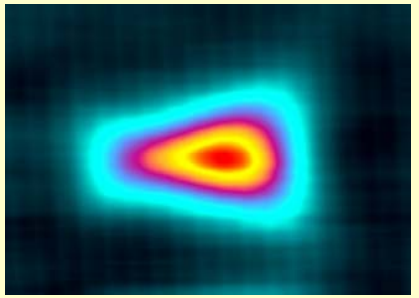
Zn in GaAs
E_b(Zn) = 30meV
a_0 = 1.8nm



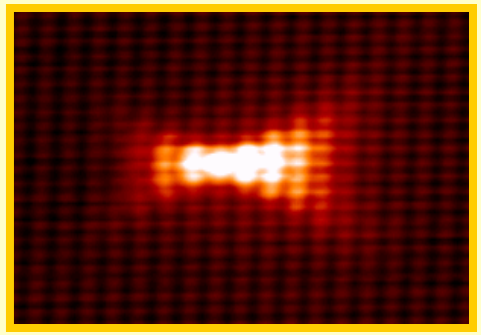


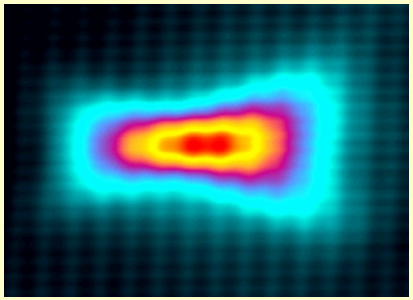
Zn in GaP
E_b(Zn) = 70meV
a_0 =~ ***0.6nm !***





Mn in GaAs
E_b(Mn) = 110meV
a_0 = 1nm





Symmetry of Impurities

Mn in GaAs | *Zn in GaP* | *Zn in GaAs*

O_8

A

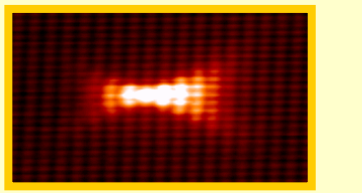
T_2

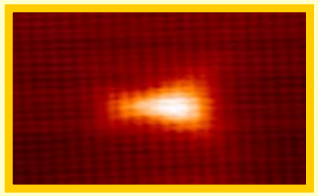
E

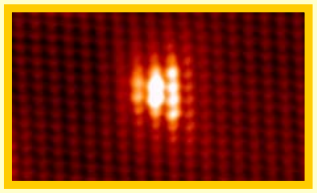
A′

T'_2

E′





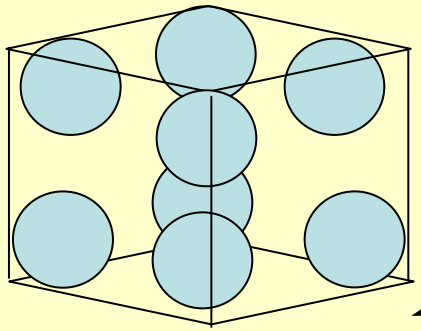


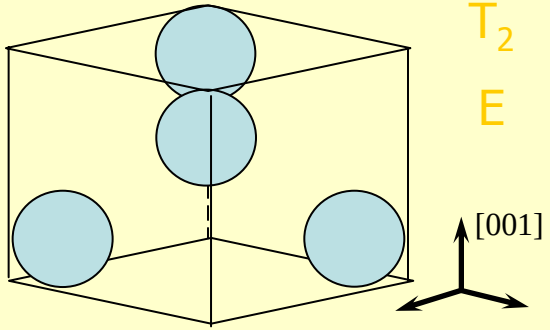
T_d

A

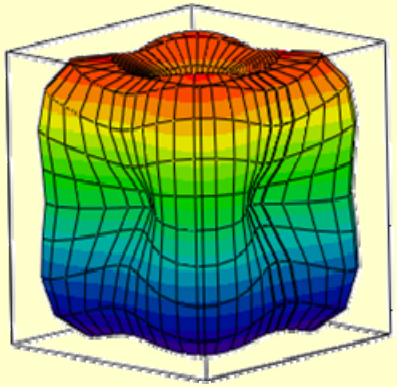
T_2

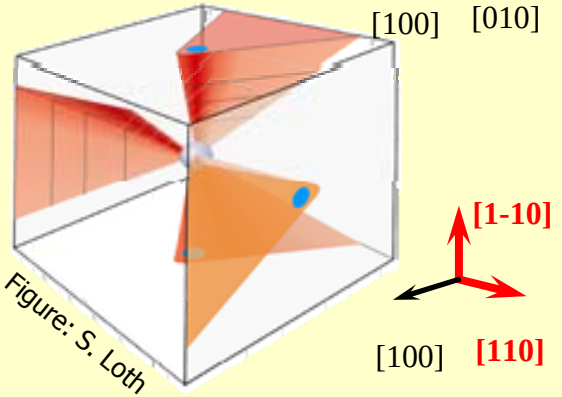
E





Effective mass
Tight binding
Ab-initio modelling





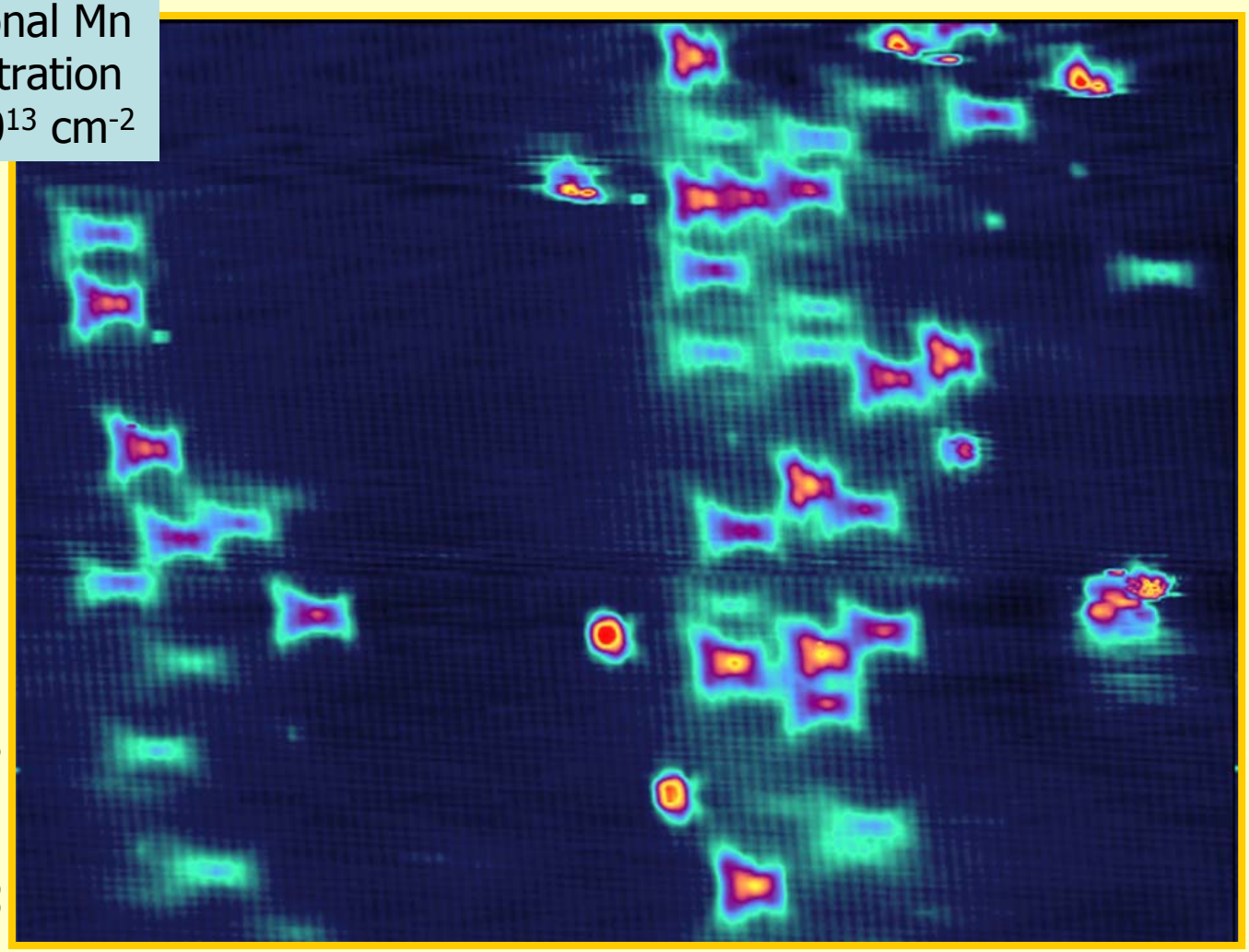
*Yakunin et al. PRL **92**, 216806 (2004)*

*S. Loth et al. PRL **96**, 066403 (2005)*
*Mathieu et al. PRL **94**, 026407 (2005)*

Pairs of magnetic impurities

Mn-delta Doped Layers

Intentional Mn concentration $N=3\times10^{13}$ cm^{-2}

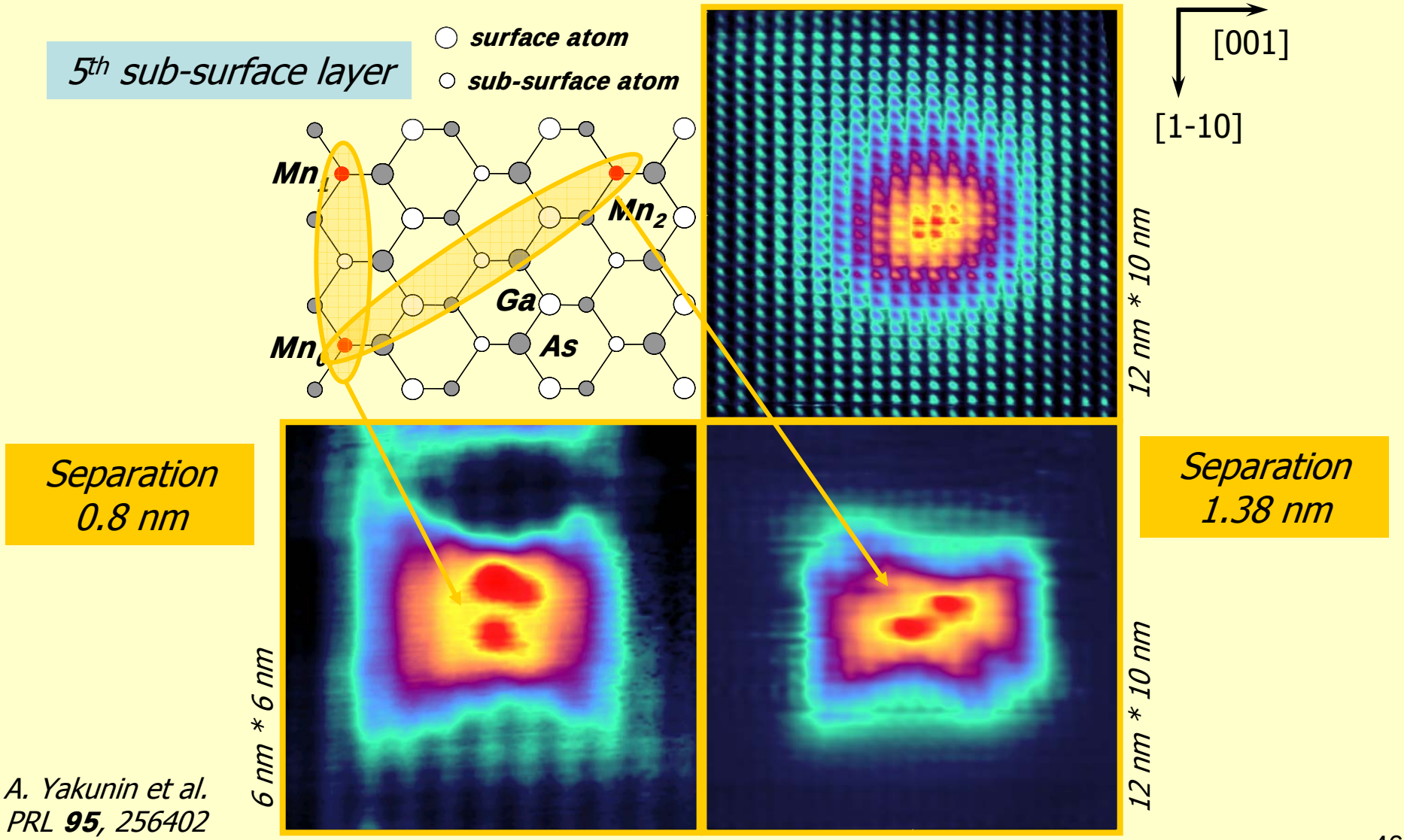


*53 nm * 40 nm*

Growth direction → [001]

Grown by J. De Boeck et al., IMEC, Belgium

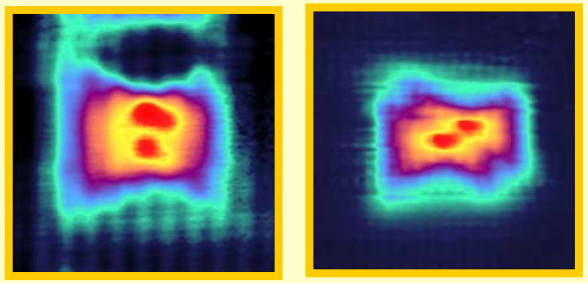
Interacting Impurities



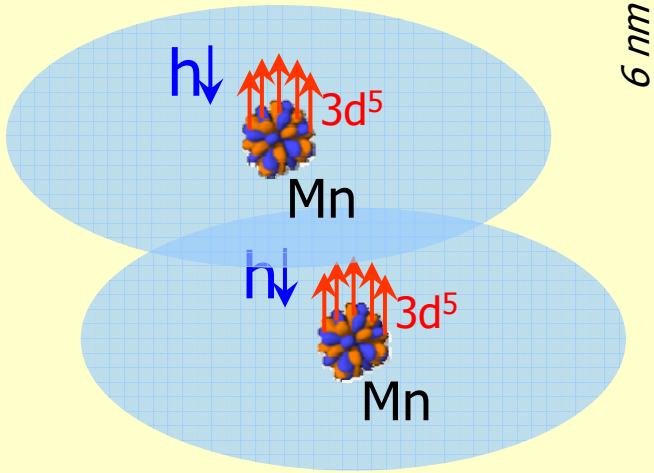
A. Yakunin et al. PRL **95**, 256402 (2005)

Grown by J. De Boeck et al., IMEC, Belgium

Experimental



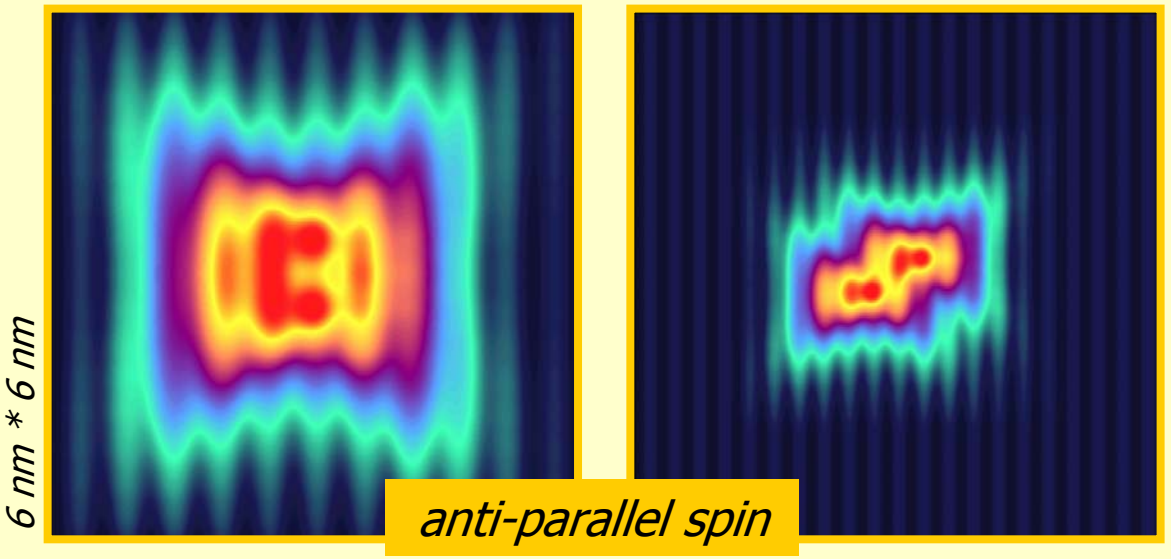
0.8 nm 1.4 nm

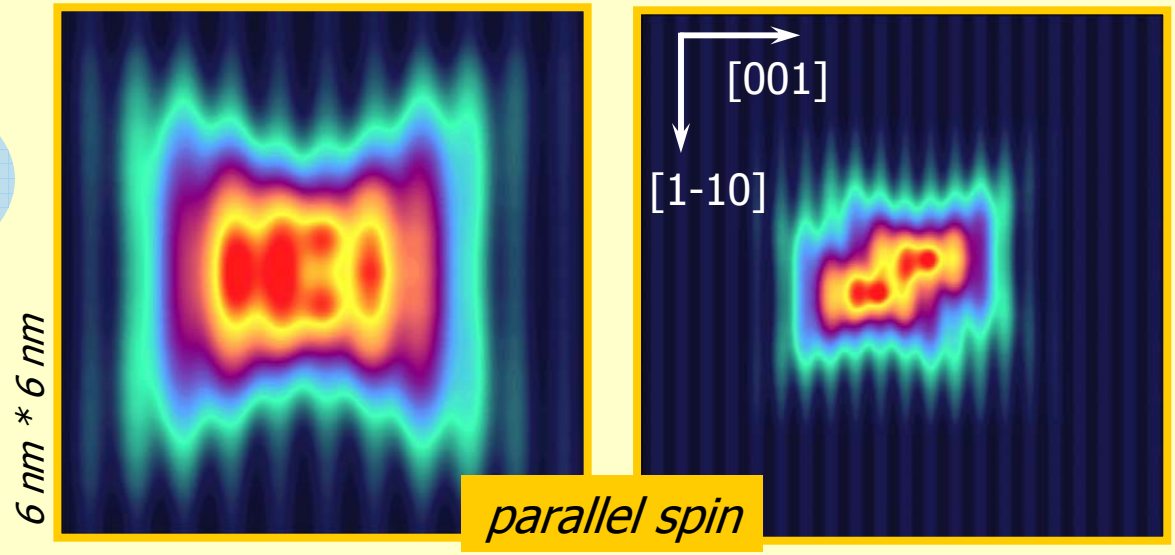


J.-M. Tang M. Flatté
Iowa, US

*A. Yakunin PRL **95**, 256402 (2005)*

TBM Simulation

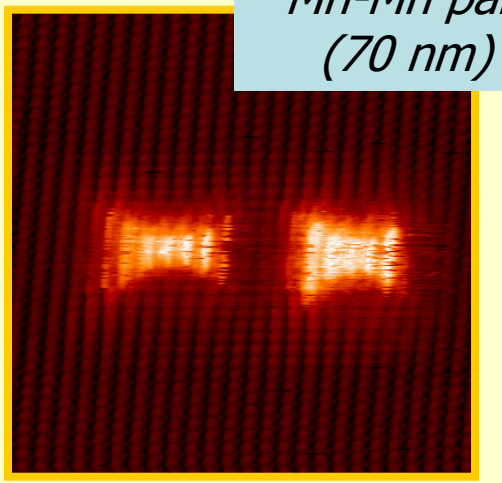




Delta layers

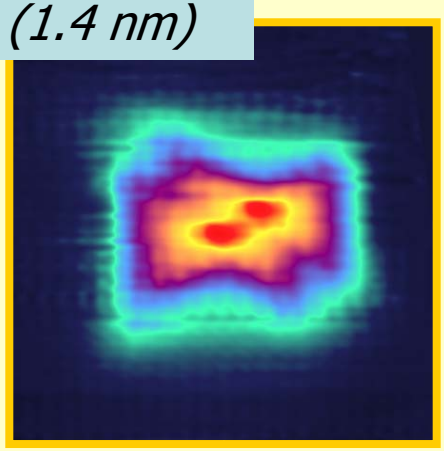
Impurity-Impurity Interaction

Mn-Mn pair (70 nm)



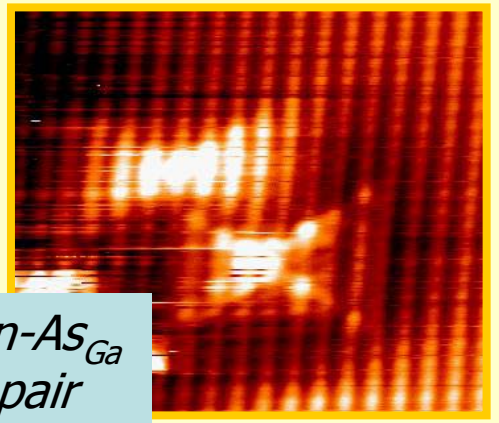
*140 nm * 140 nm*

Mn-Mn pair (1.4 nm)



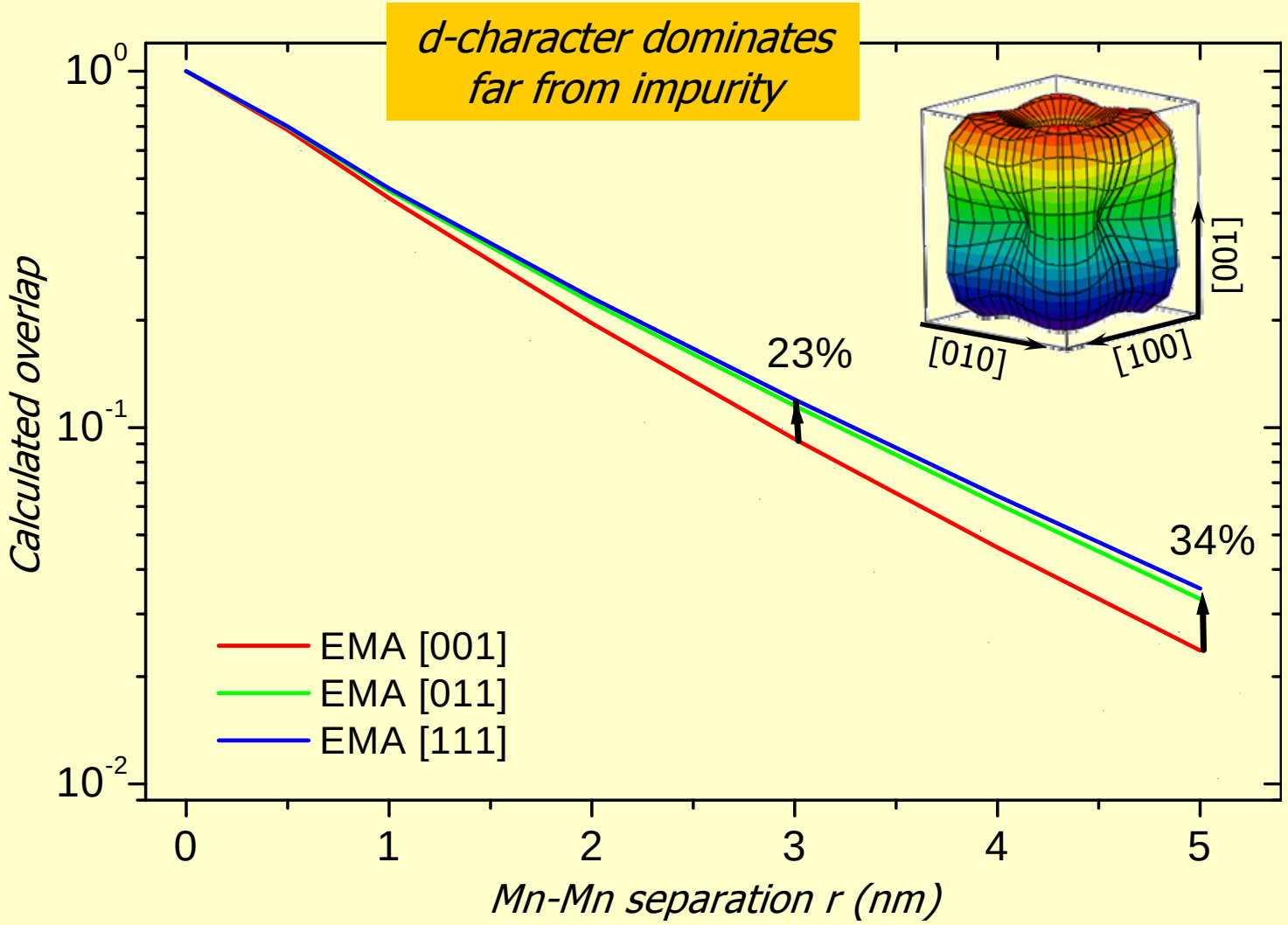
*12 nm * 10 nm*

Mn-As$_{Ga}$ pair

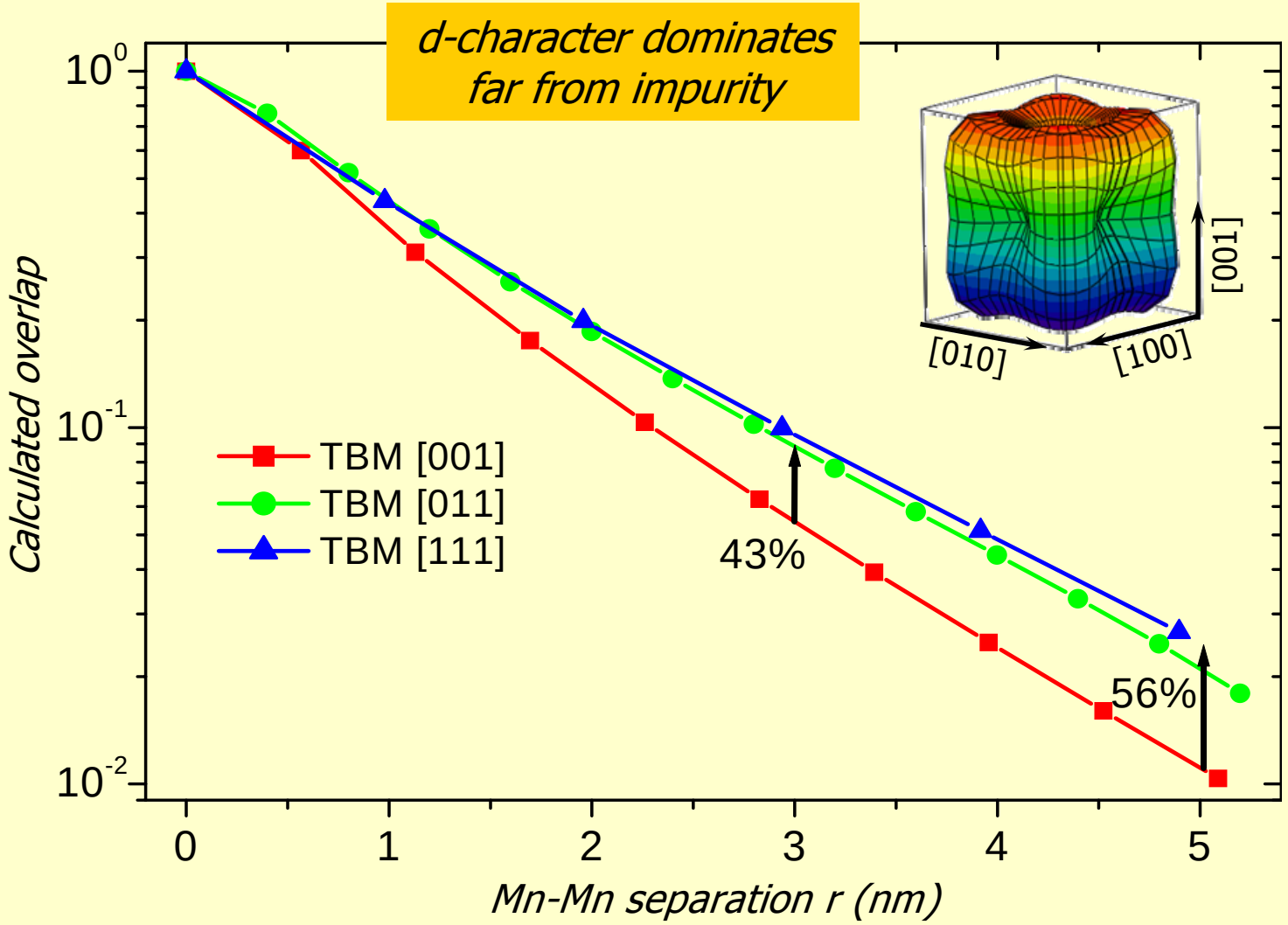


*60 nm * 80 nm*

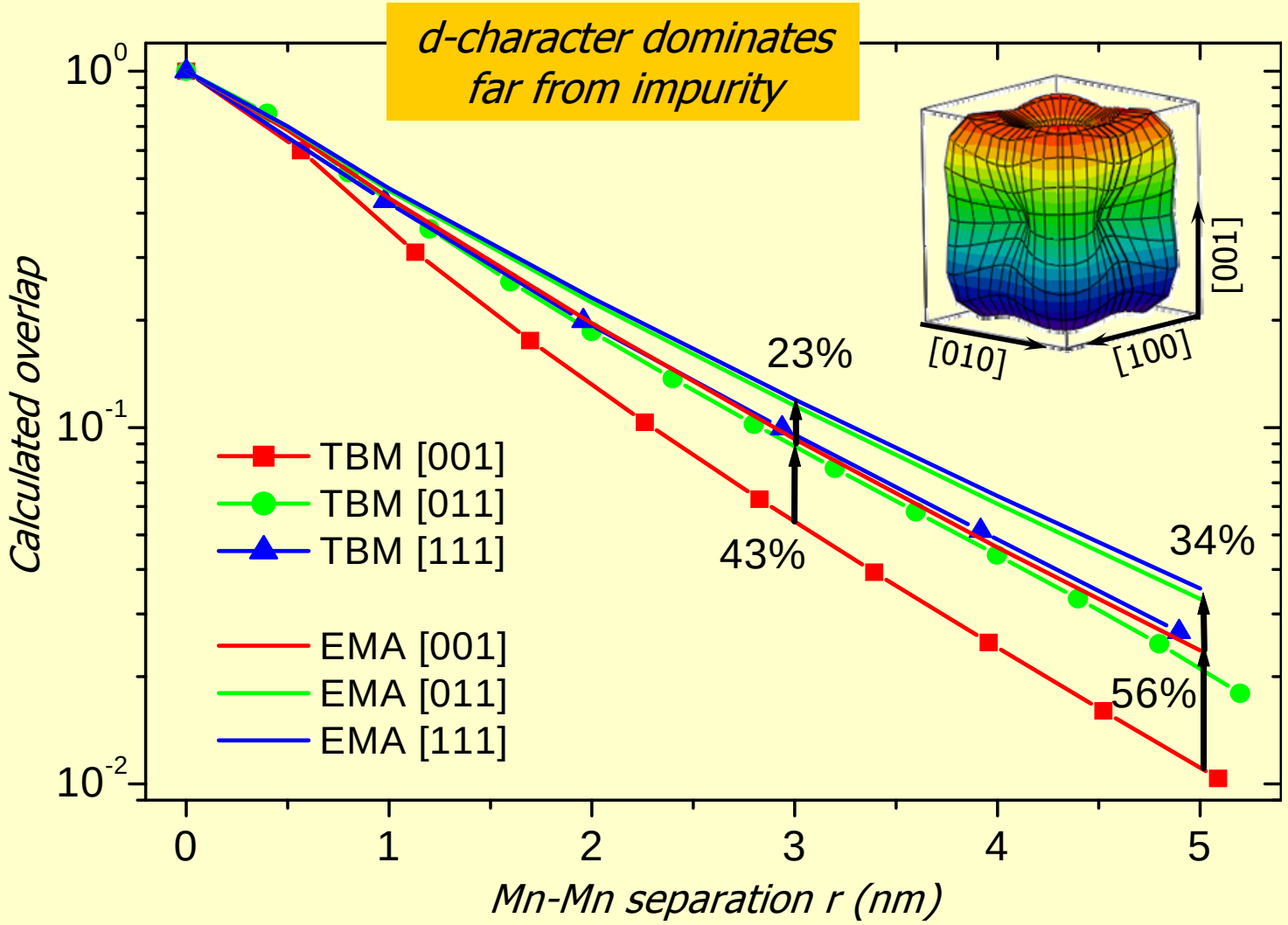
Directional Dependence Mn-overlap



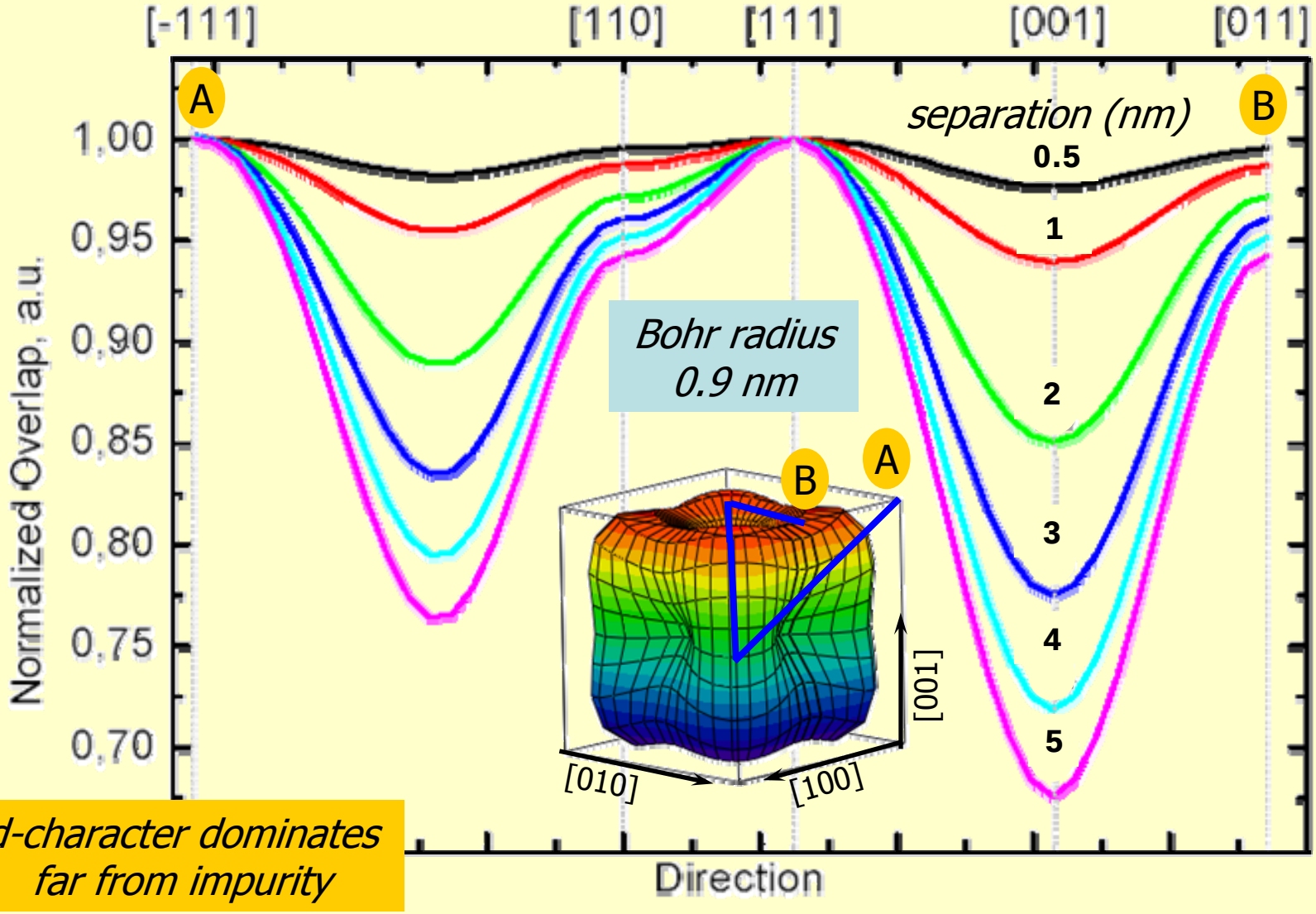
Directional Dependence Mn-overlap



Directional Dependence Mn-overlap

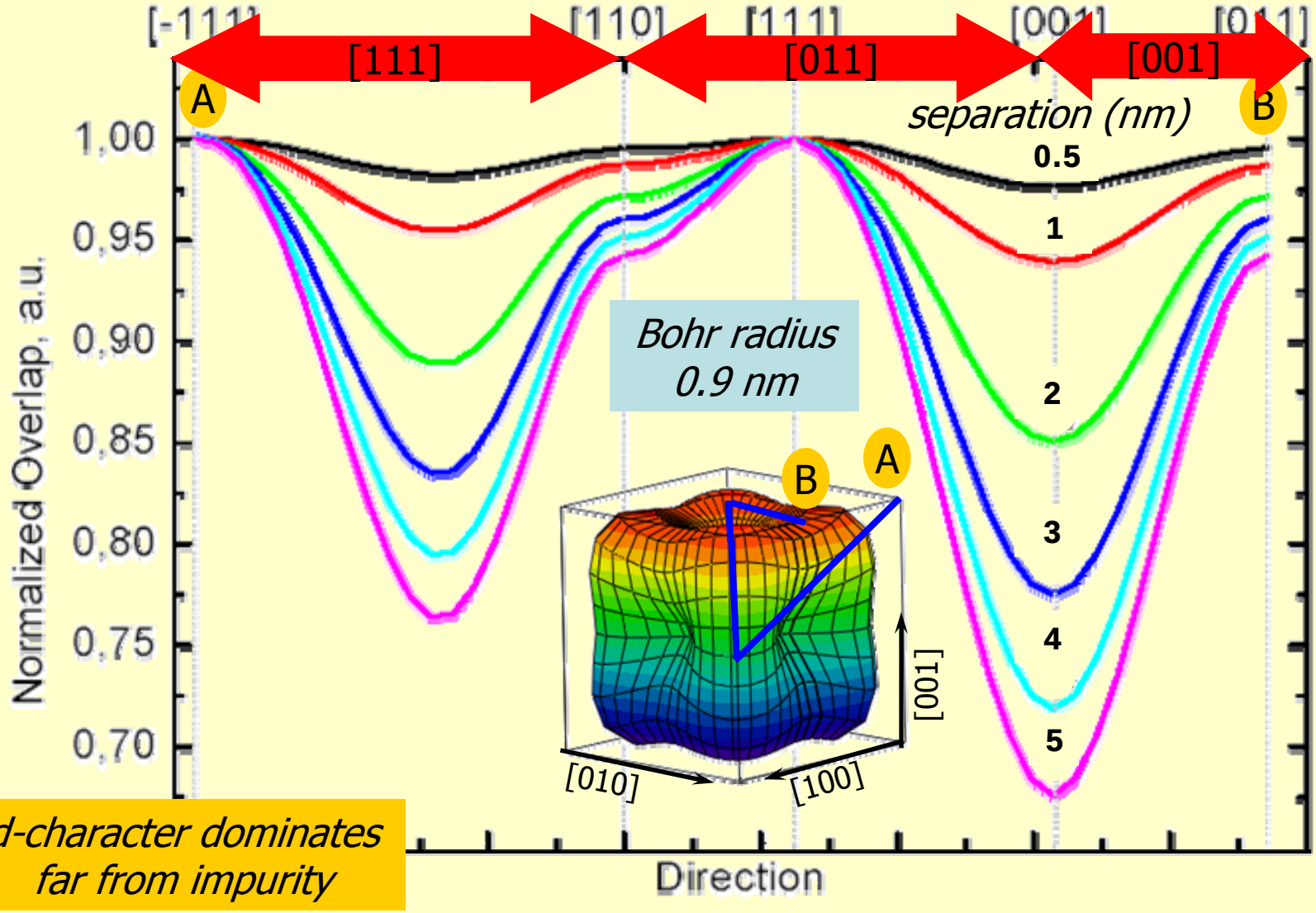


Directional Dependence Mn-overlap



d-character dominates far from impurity

Directional Dependence Mn-overlap



d-character dominates far from impurity

Overlap Expectation on [i,j,k] Plane

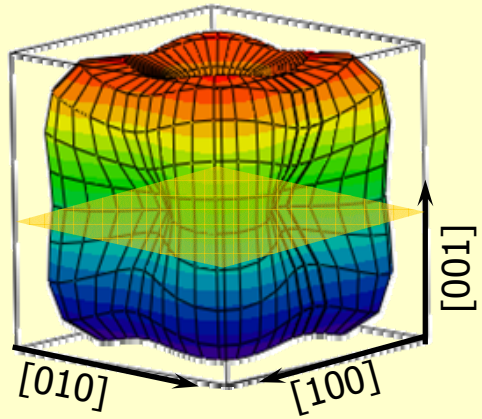
$4*10^{14}$ cm^{-2} (100%)

$4*10^{12}$ cm^{-2} (1%)

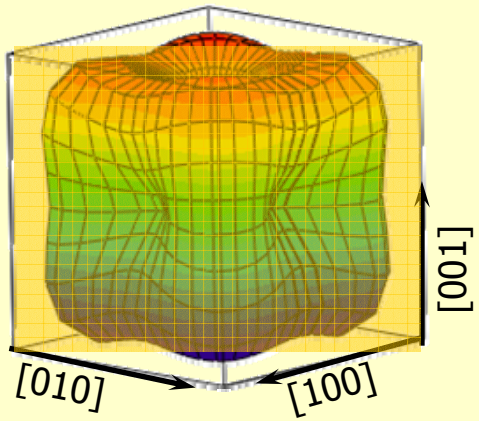
r(Å)	N	$\Omega^{(001)}$	$\Omega^{(110)}$	$\Omega^{(111)}$
5	0.654	0.986	0.990	0.992
10	0.438	0.963	0.976	0.980
20	0.216	0.912	0.941	0.952
30	0.112	0.870	0.913	0.929
40	0.060	0.837	0.892	0.912
50	0.033	0.812	0.875	0.898

Highest T_{curie} on the [111] doping plane ?

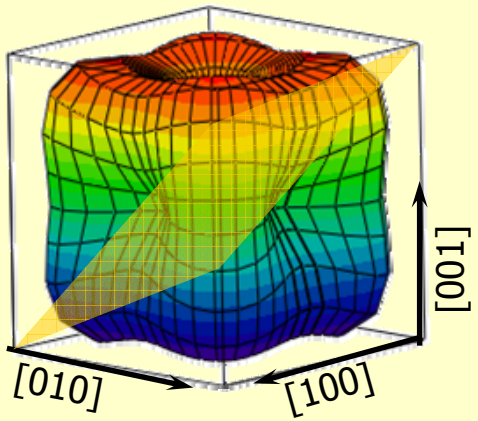
[001] doping plane



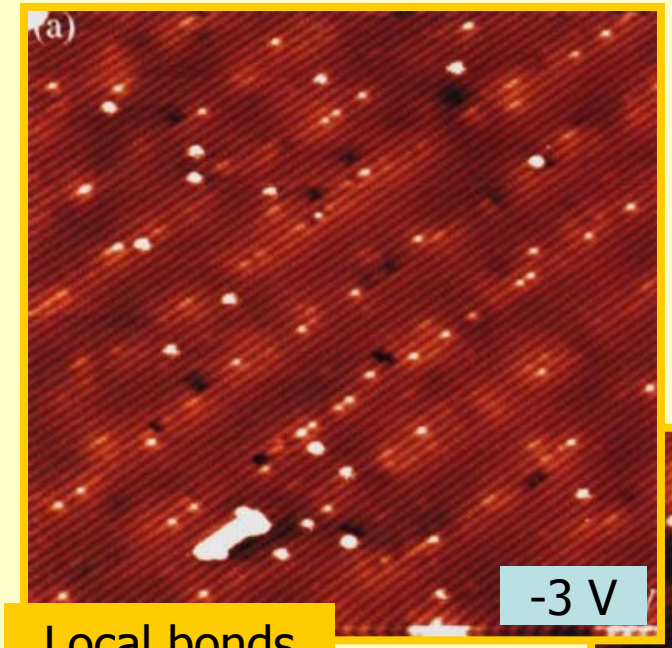
[011] doping plane



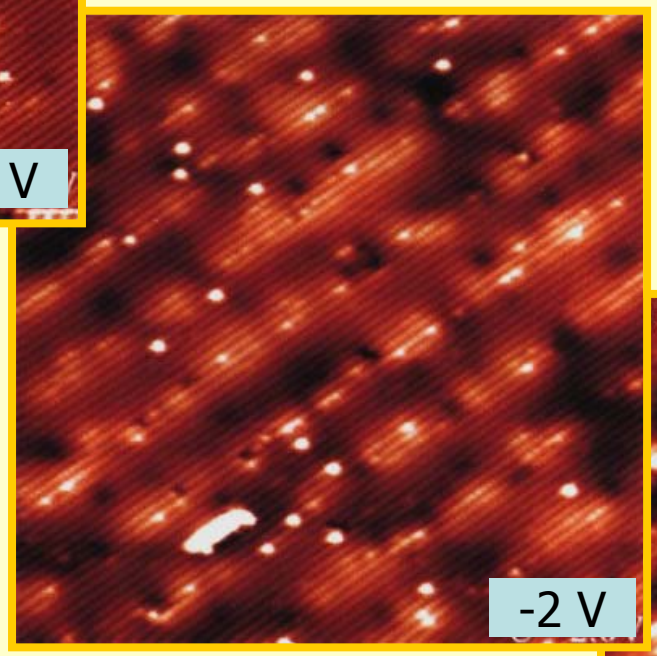
[111] doping plane



High Concentration Mn Delta Layers



Local bonds surface Mn

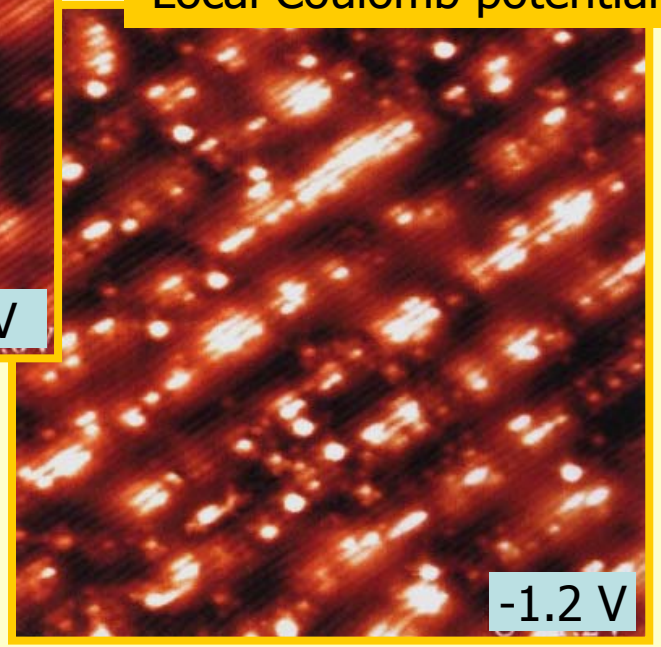


*35 nm * 35 nm*

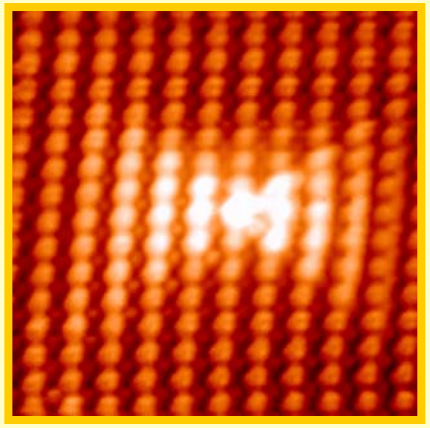
Grown at PDI, Berlin, Germany

Mn in ionized state

Local Coulomb potential



$Ga_{0.8}Mn_{0.2}As$ delta layers
($1*10^{14}$ cm^{-2})



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