Atomistic understanding of transport through a single dopant atom in a MOSFET

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EU/FET Cluster meeting
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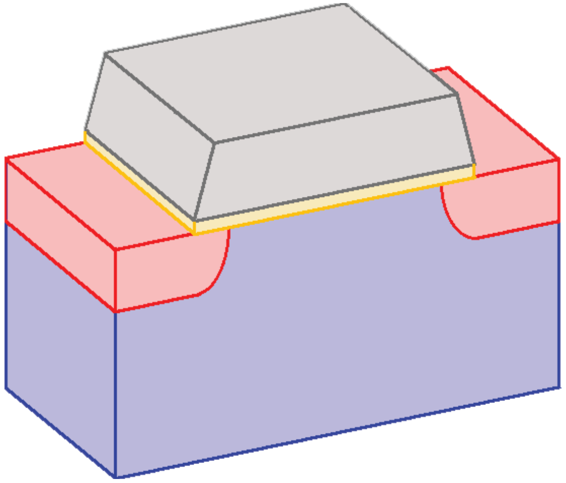
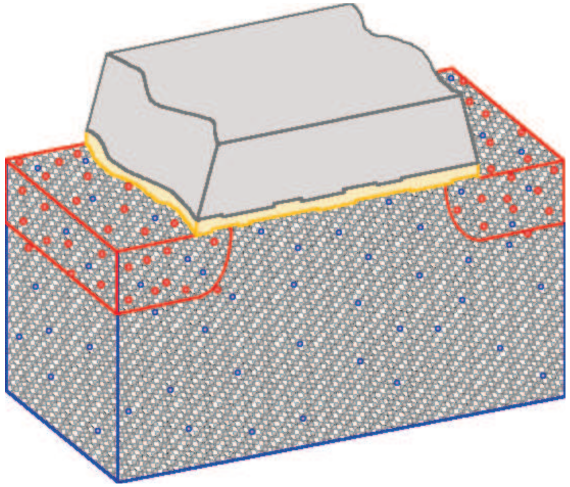
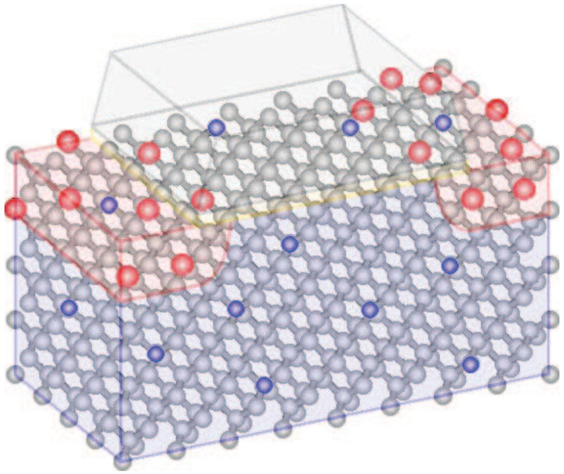
Atomic-scale electronics



“bulk” transistor (FET)



32 nm MOSFET

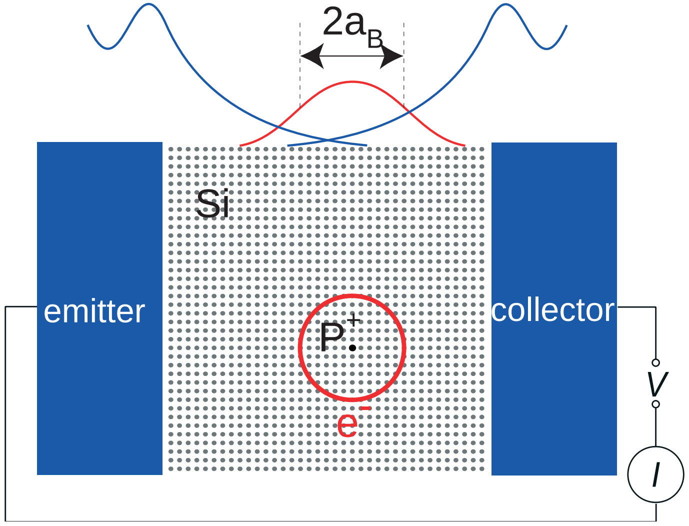


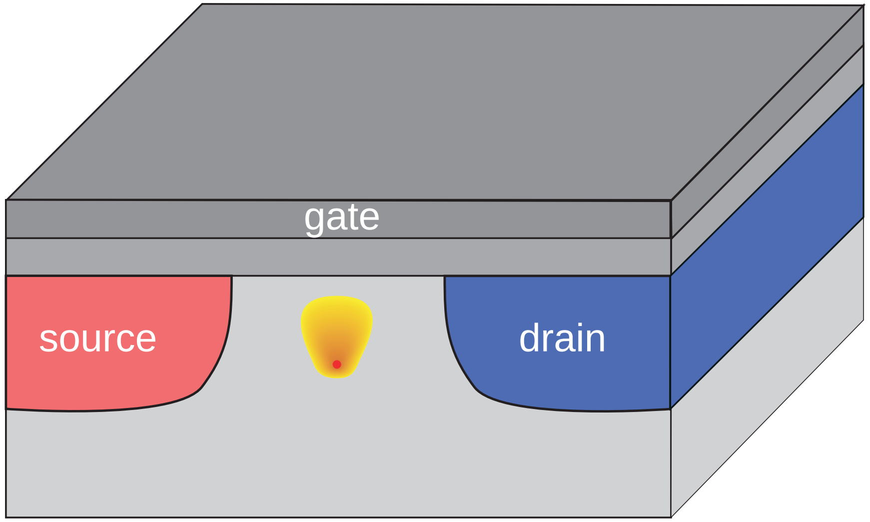
4 nm MOSFET ???

[Asenov IEEE Trans. Elec. Dev. 50, 1837, 2003]

bulk → atomistic: a *problem* for industry, an *opportunity* for science

Opportunity: Use atomic nature of a dopant for new functionality





Scaling of the Bohr orbit:

$$\begin{aligned} r_{\text{dopant}} &= \frac{\epsilon_{\text{r}}}{m^*} \cdot r_{\text{Hydrogen}} \\ r_{\text{Hydrogen}} &= 0.05\,\text{nm} \\ r_{\text{P:Si}} &= 2.5\,\text{nm} \\ r_{\text{P:Ge}} &= 6.4\,\text{nm} \end{aligned}$$

Physics of a single atom in a solid state matrix

- smallest length scale of a semiconductor device
- FET based on atomic orbitals
- 300 K quantum devices (deeper impurities)?

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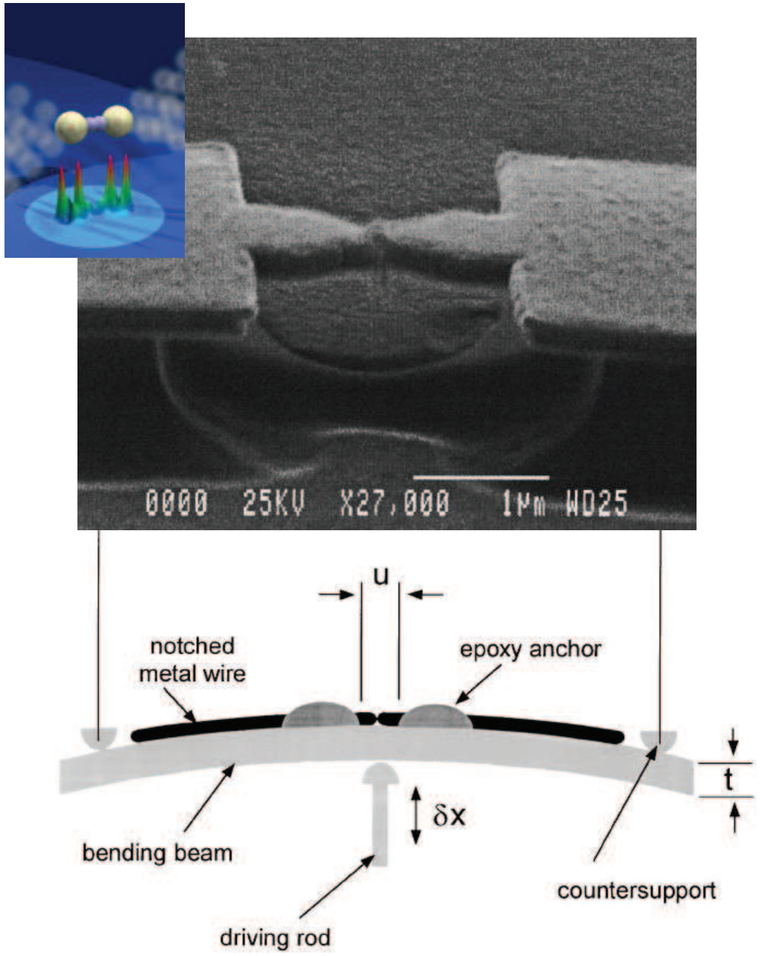
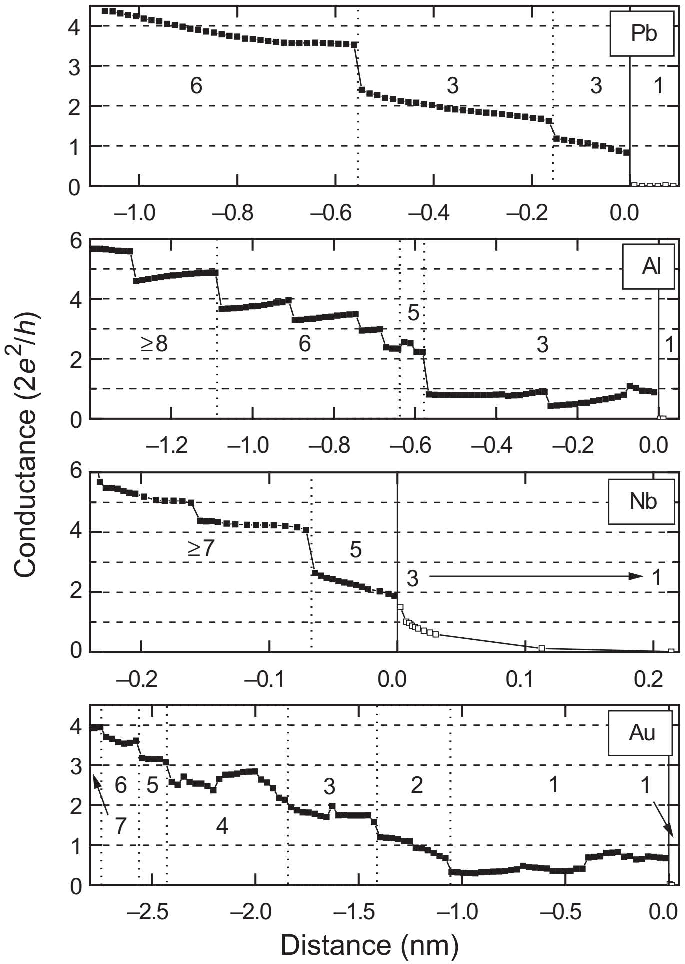
Analogy to our work: Atomic-scale electronics in a metal



transport through single metal atom in a mechanical break junction

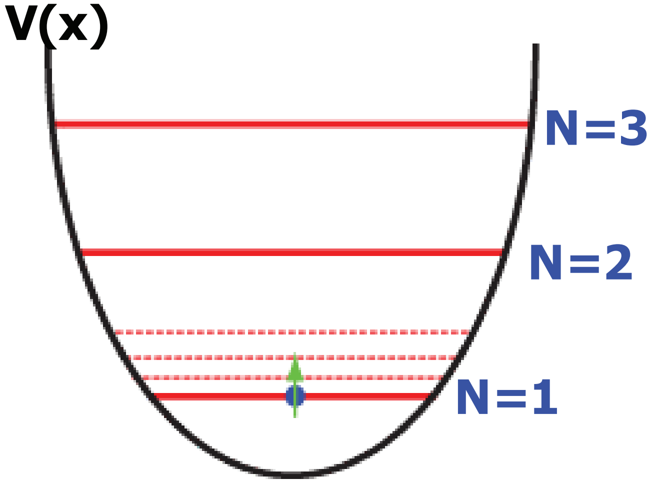


large energy scale & short length scale make it hard to realize a gate

van Ruitenbeek , RSI 67, 108, 1996 & Scheer Nature 394, 154, 1998

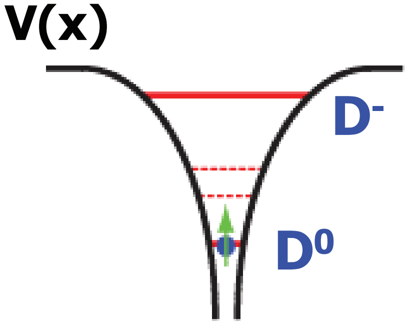
Atomic systems in a semiconductor

Quantum dots

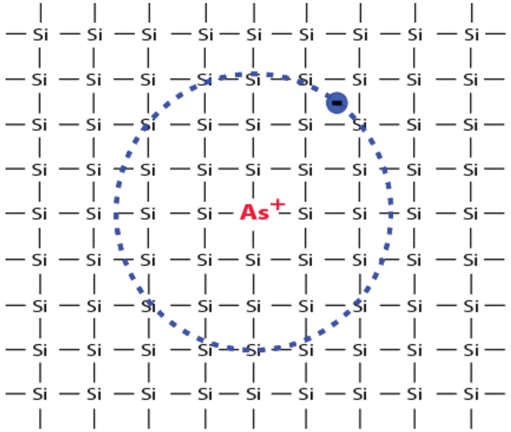


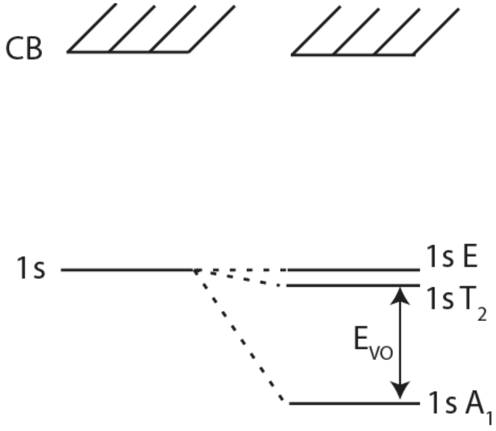
- Parabolic potential
- Constant charging energy
- Equidistant level spacing (excited states)

Dopant: shallow donors in Si

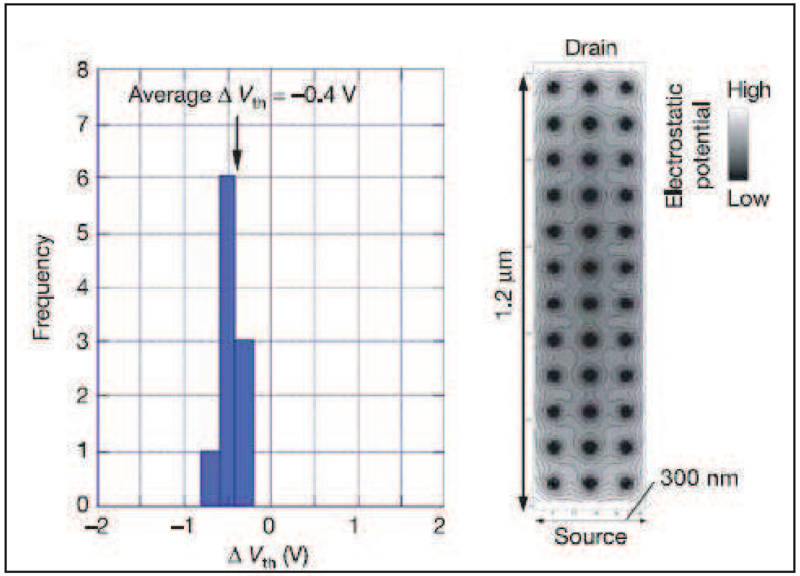


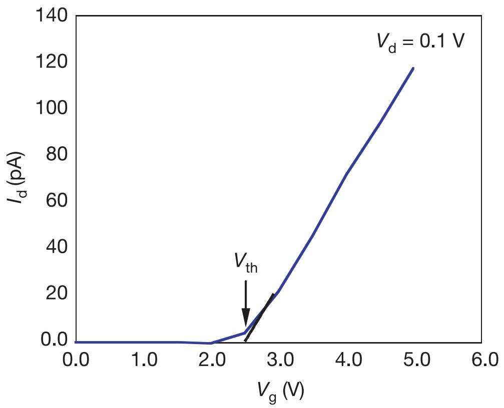
- Coulomb potential
- Can bind up to two electrons
- Hydrogen-like level spectrum (D^0)
- Valley-orbit →



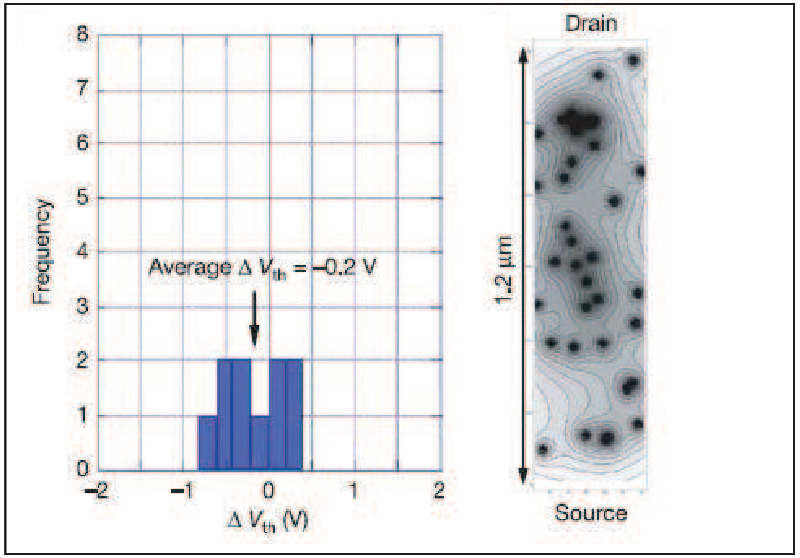


Recent progress in top-down dopant engineering

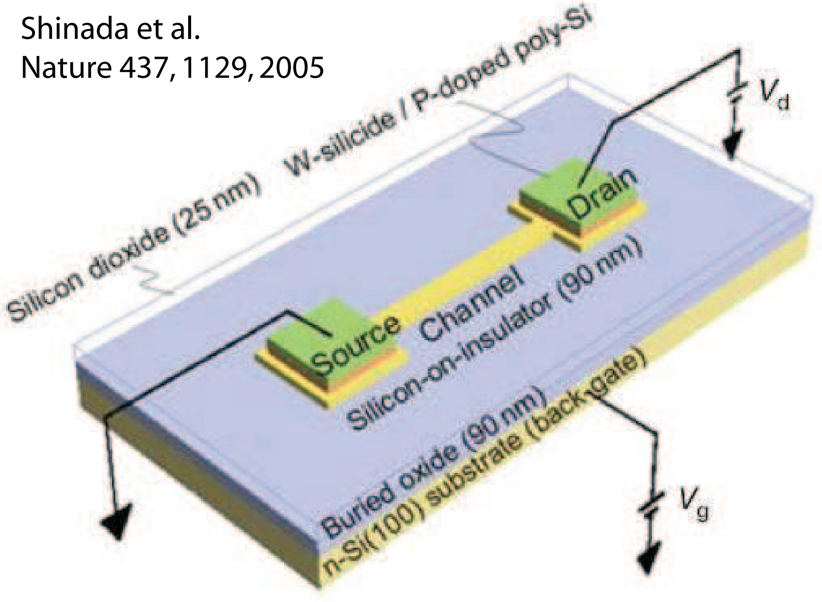




Improved V_{th} distribution due to dopant engineering

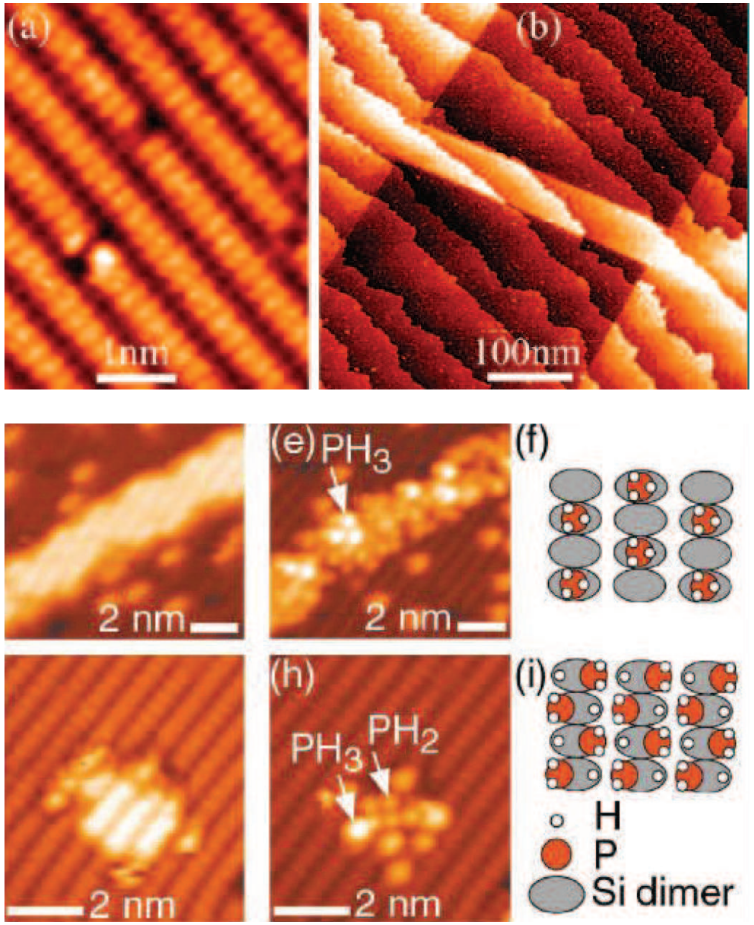


Shinada et al.
Nature 437, 1129, 2005

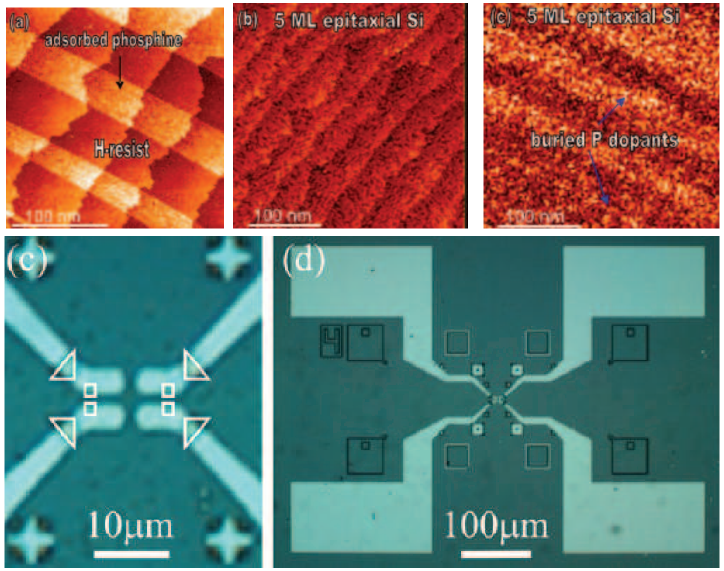


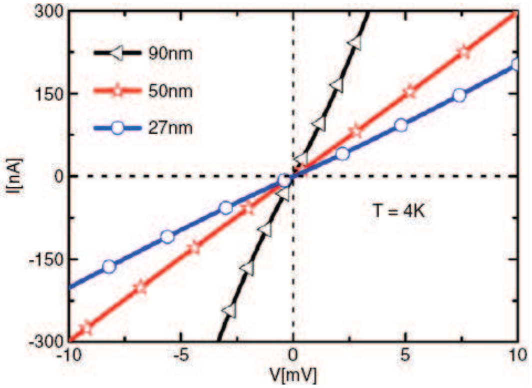
Ultimate goal: Dopant superlattice [Esaki & Tsu, IBM J. Res. Dev. '70]

Recent progress in bottom-up dopant engineering



hydrogen passivation and local desorption,
selective phosphor CVD based on PH$_3$

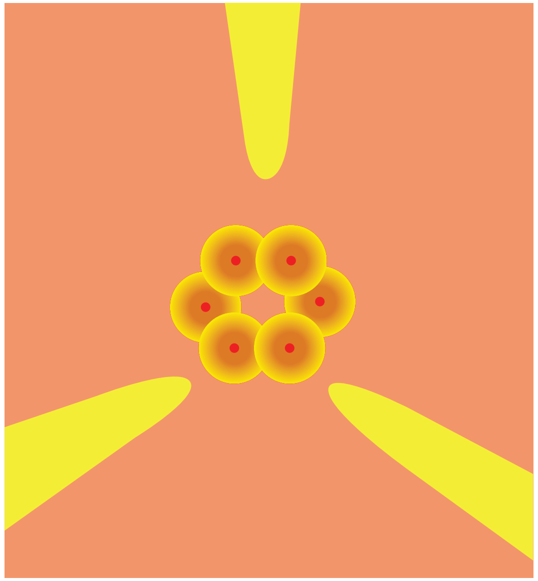




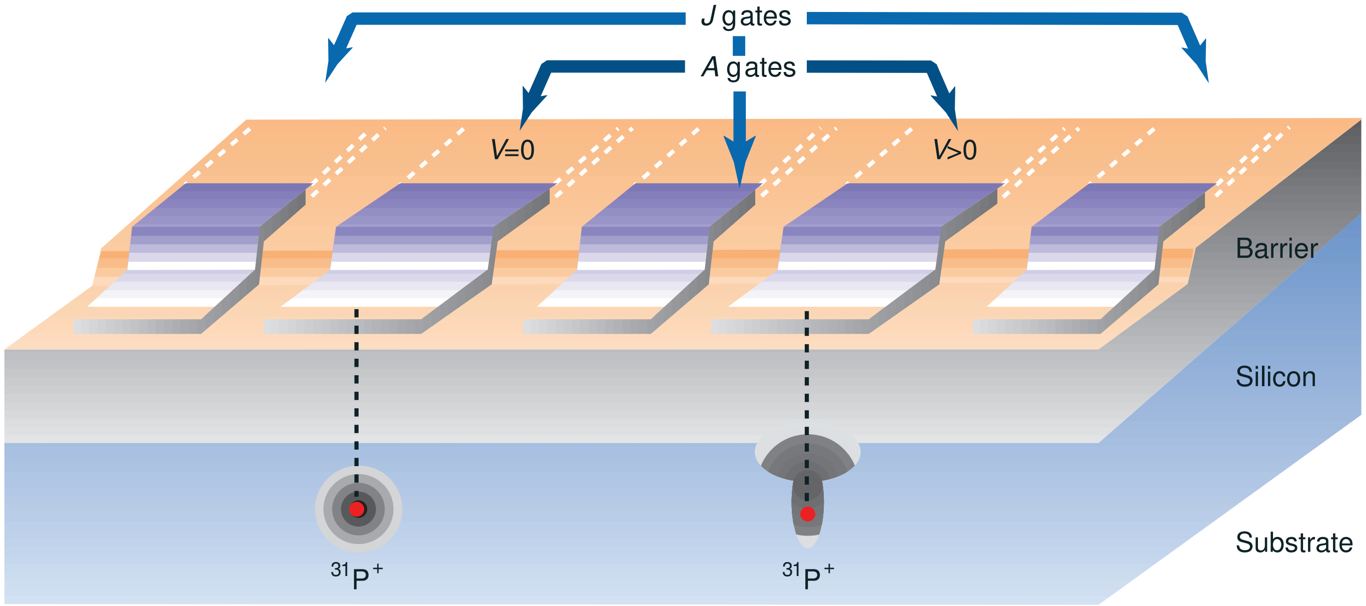
incorporation & Si overgrowth
ex situ measurements of device

Schofield, PRL 91, 136104, 2003 & Russ, Nanotech. 18, 044023, 2007

New device concepts based on atomic functionality



[molecular electronics in the solid state]

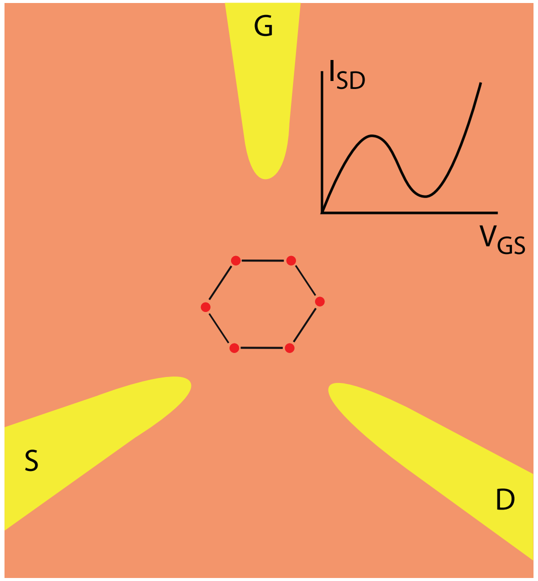


[Kane Nature 393, 133, 1998]

Devices utilizing the atomic nature of a dopant atom:

- solid-state molecules based on bound states of electrons or holes in a semiconductor
- important length scale = Bohr orbit → addressable via gate control
- quantum coherent devices: Si/Ge attractive due to long spin coherence times

New device concepts based on atomic functionality



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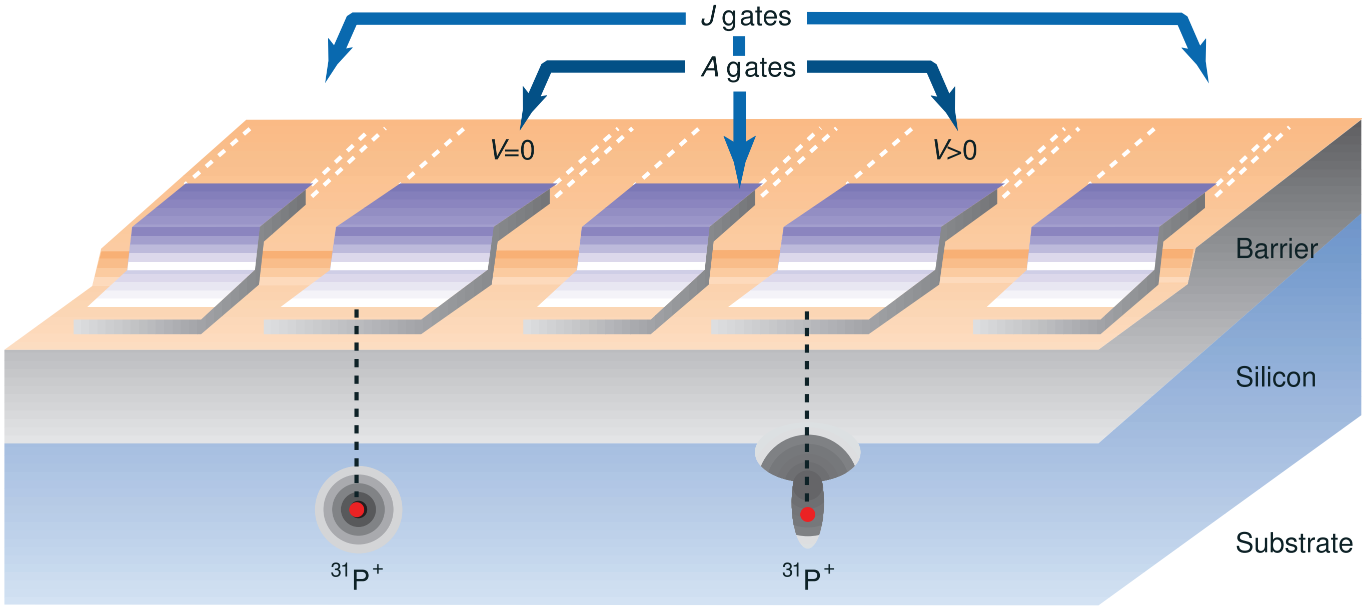

[Kane Nature 393, 133, 1998]

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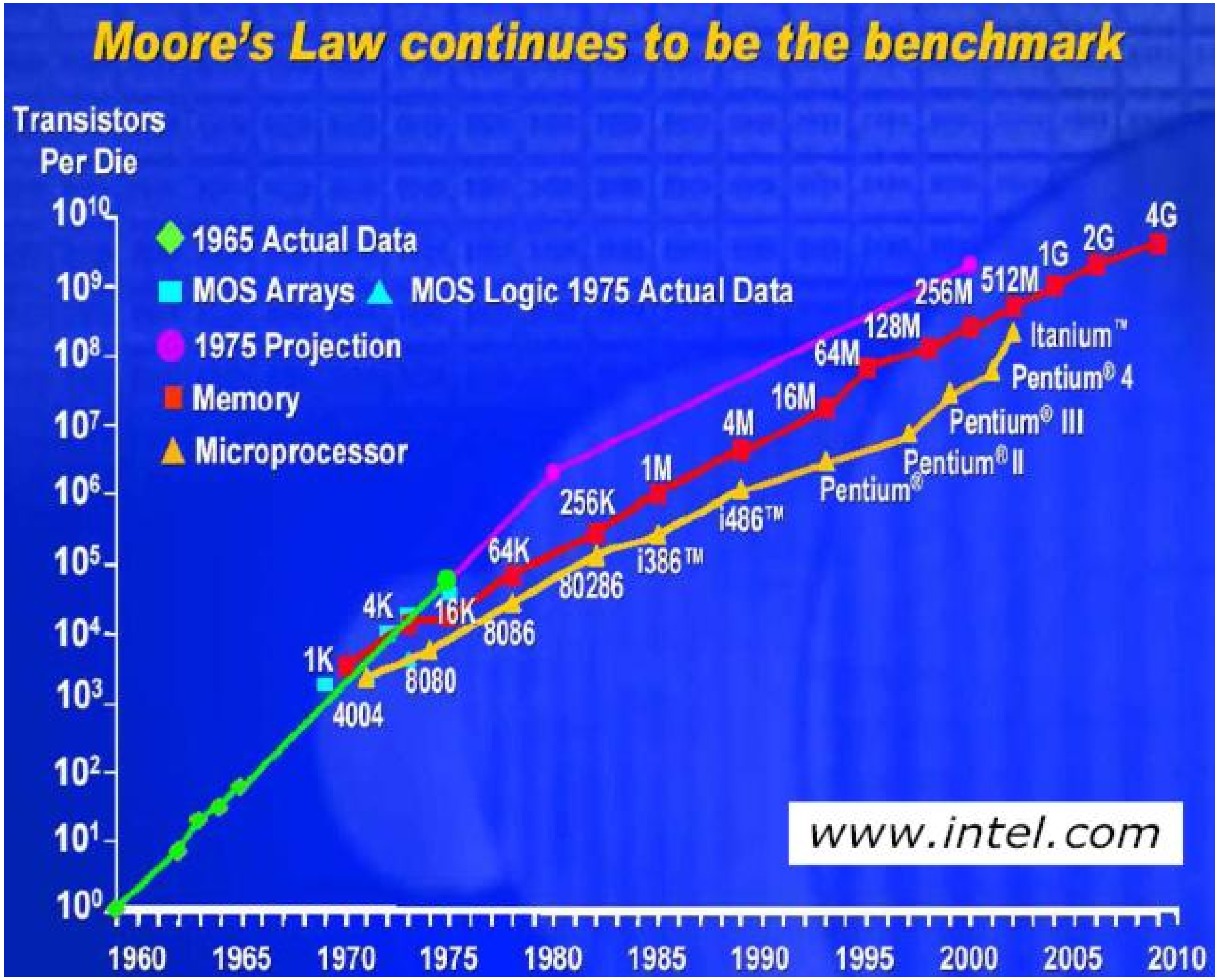
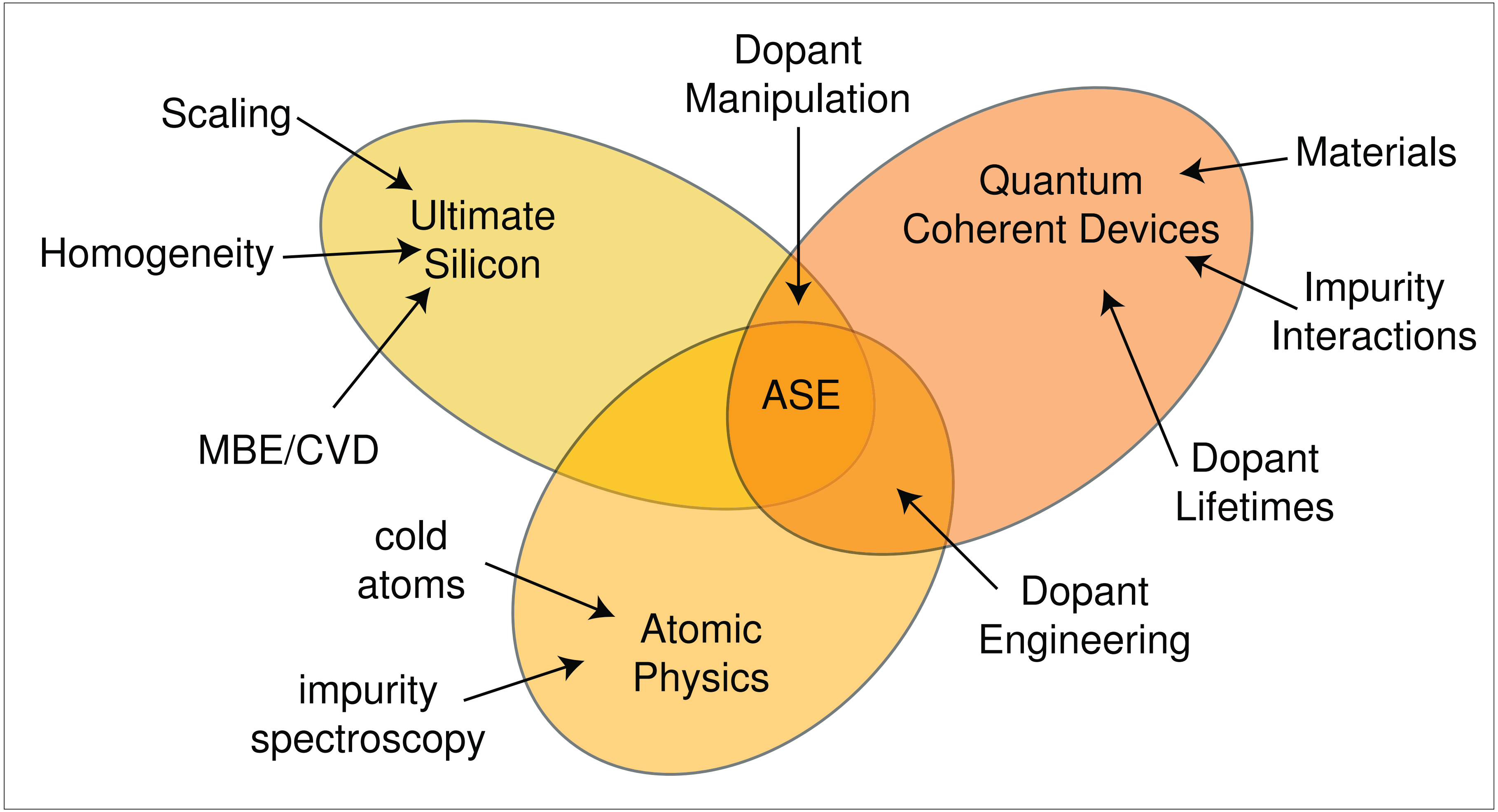
New functionality in CMOS at the end of the roadmap



use ultimate CMOS technology to achieve new functionality in this material system

Atomic-scale electronics



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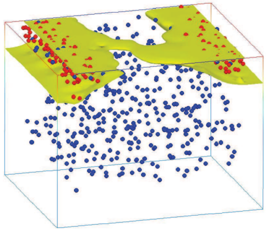
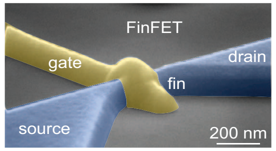
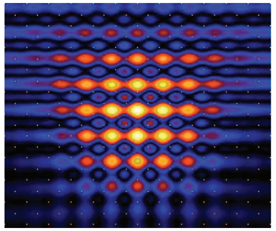
Outline



- Atomic-scale electronics



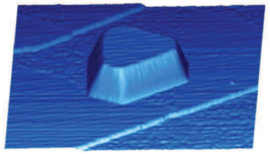
- Access to a single dopant in a nano-MOSFET



- Atomic physics in a MOSFET

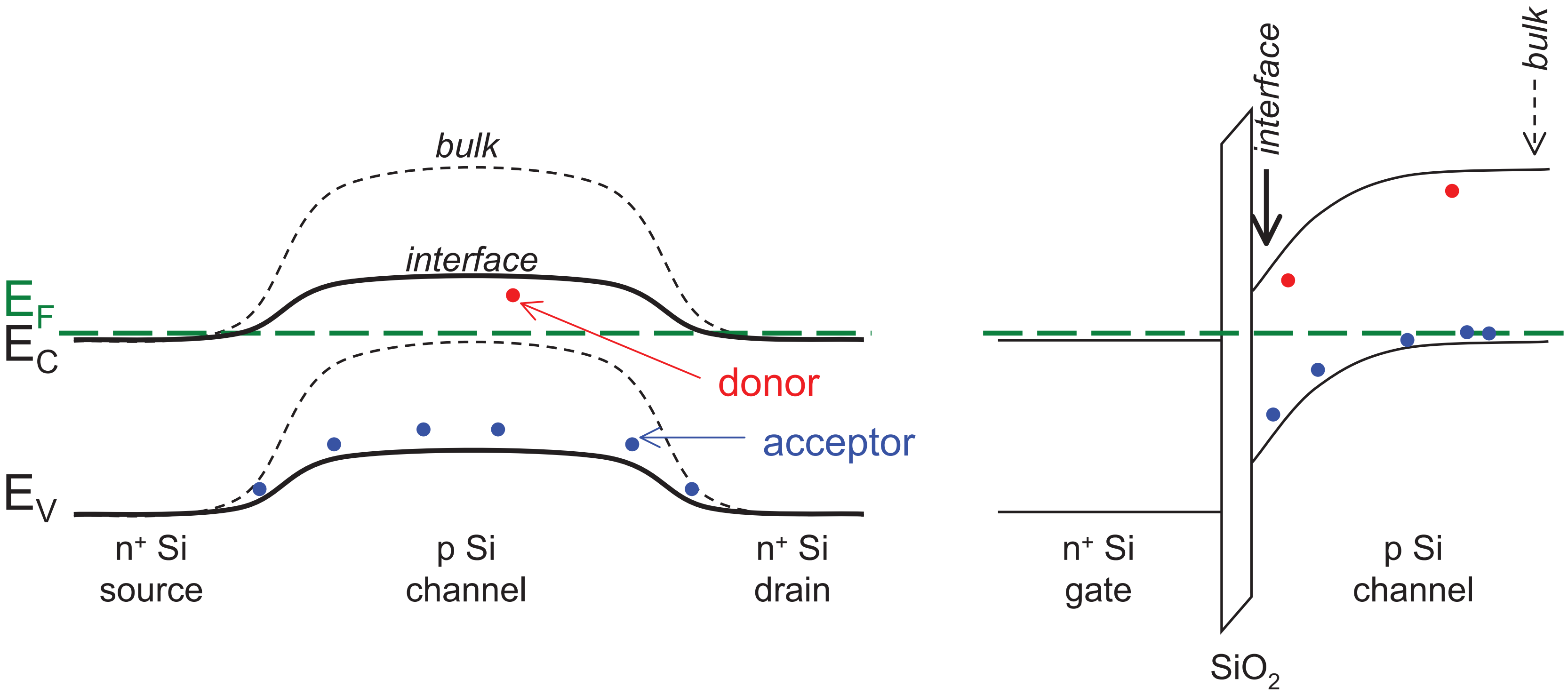
Σ

- Summary



- Other projects

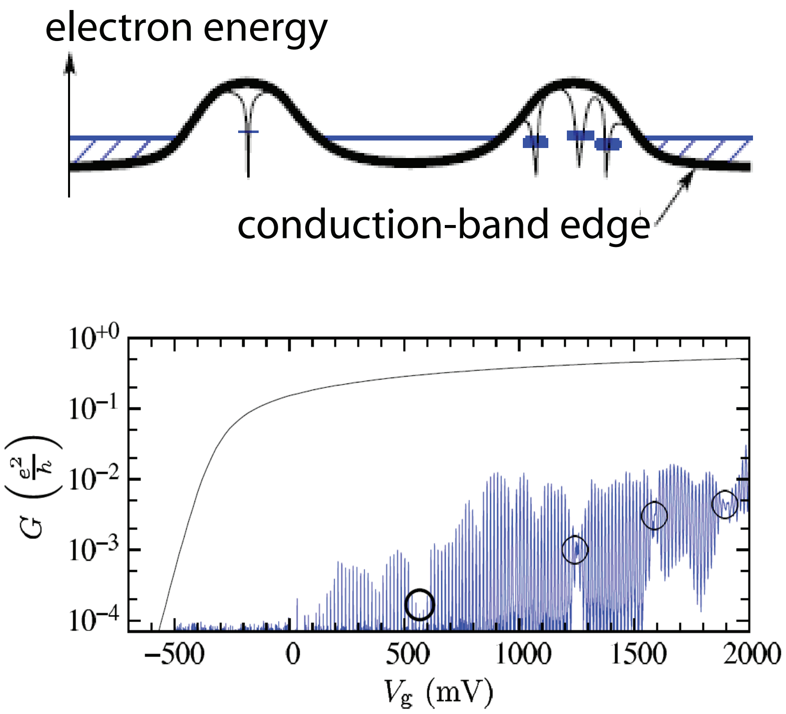
How many dopants are in a FET?



- How many dopants are there?
  - N(acceptors) $= 10^{18}/\text{cm}^3 \times (60 \times 60 \times 35\text{nm}^3) \approx 125$
  - N(acceptors in resonance) $= (60+60+35\text{nm})/(10^{18}/\text{cm}^3)^{1/3} \approx 15$
  - N(donors)= less than acceptors → may be observed individually
- Which dopants are probed?
  - acceptors: require interband tunneling → no
  - donors: subthreshold current at interface → yes

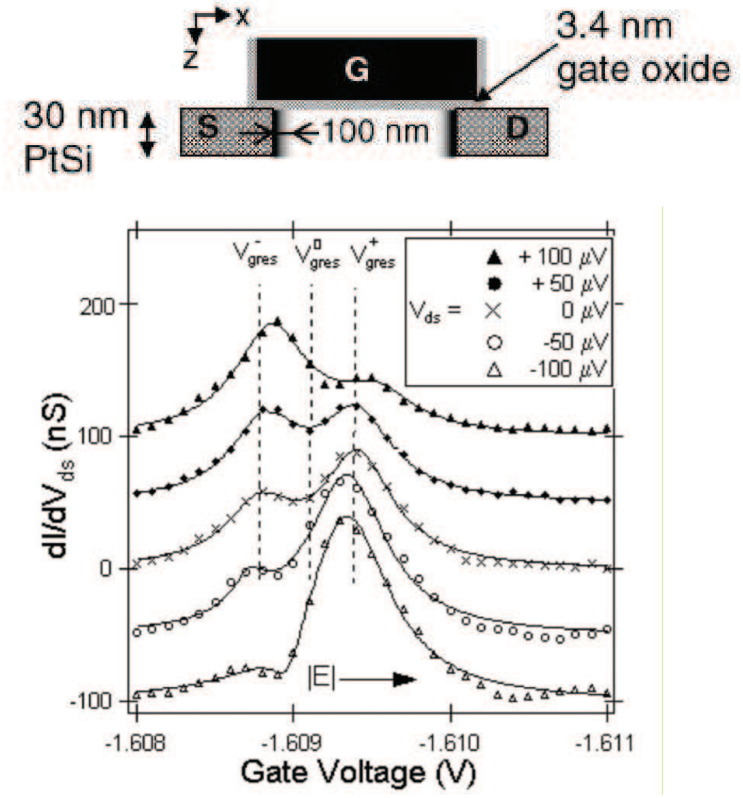
Transport through dopants in a MOSFET

M. Hofheinz et al., Eur. Phys. J. B 54, 299–307 (2006)



dopants in the access regions of a MOSFET

L. Calvet et al., PRL 98, 096805 (2007)



dopants between source and gate of a Schottky transistor

strong recent interest in transport through dopants but not with dopants in the channel

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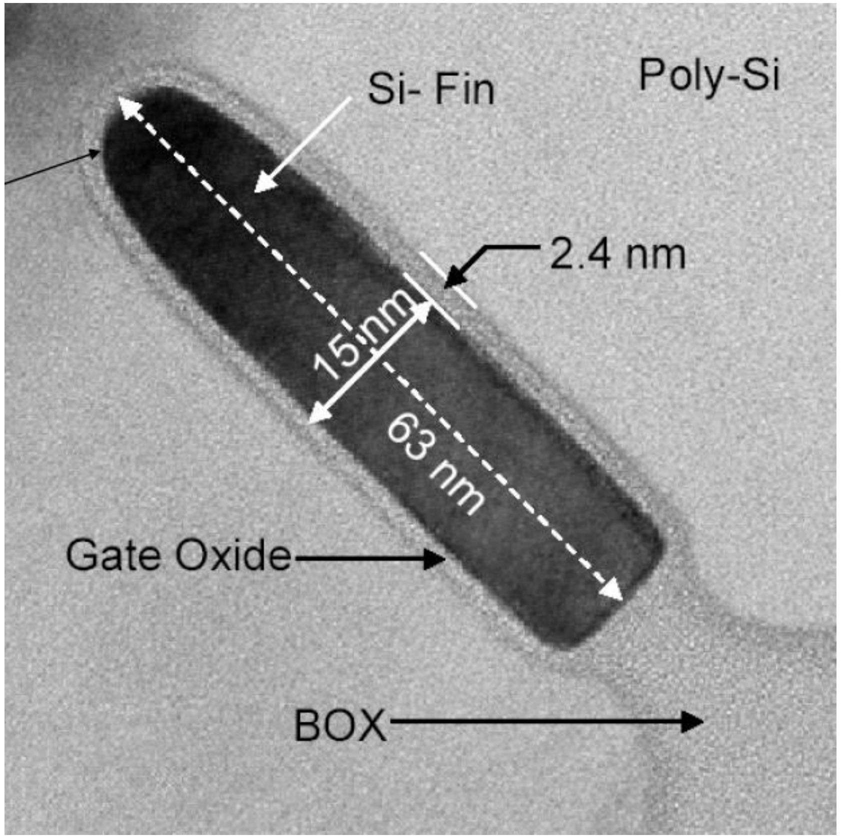
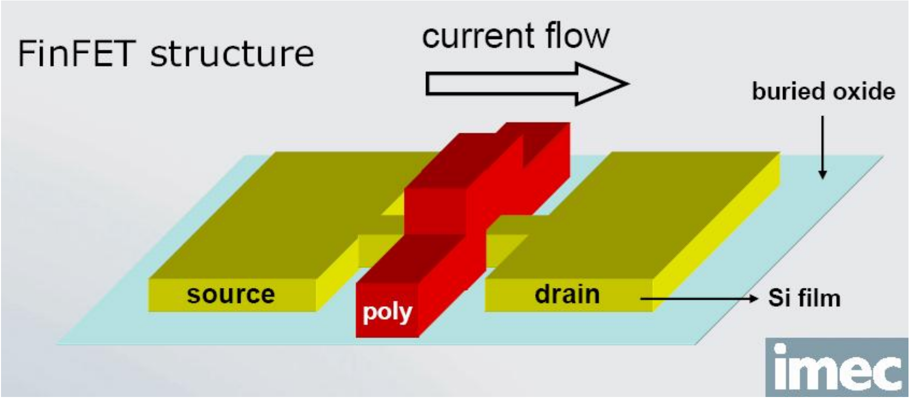
Multi-gate FET (FinFET) from S. Biesemans group (IMEC)

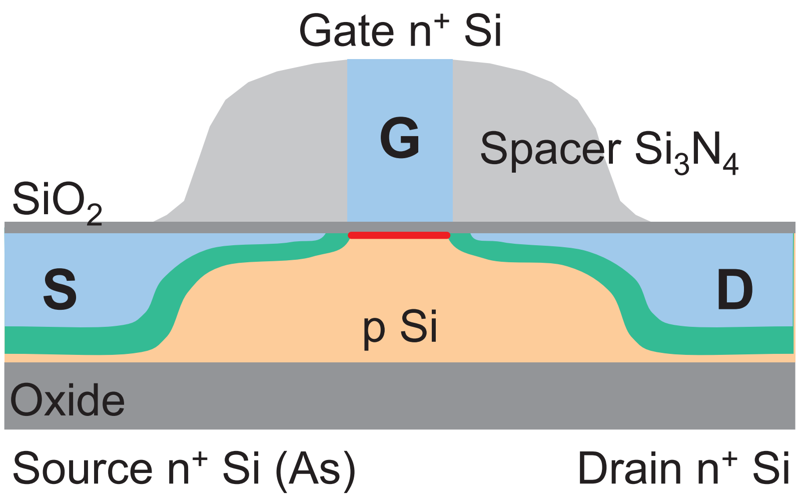


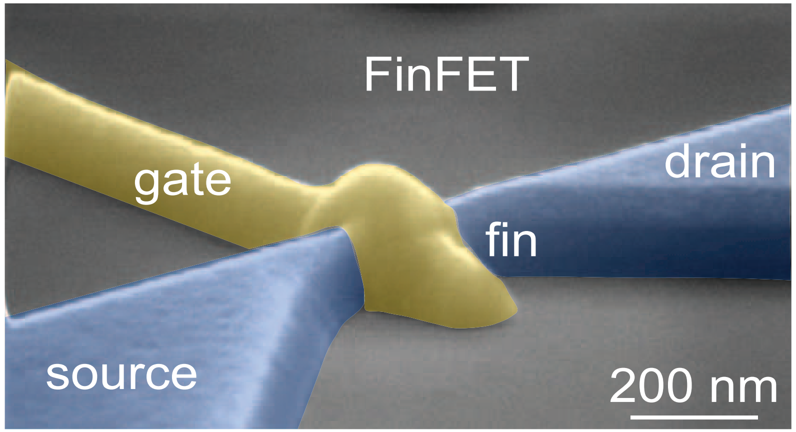


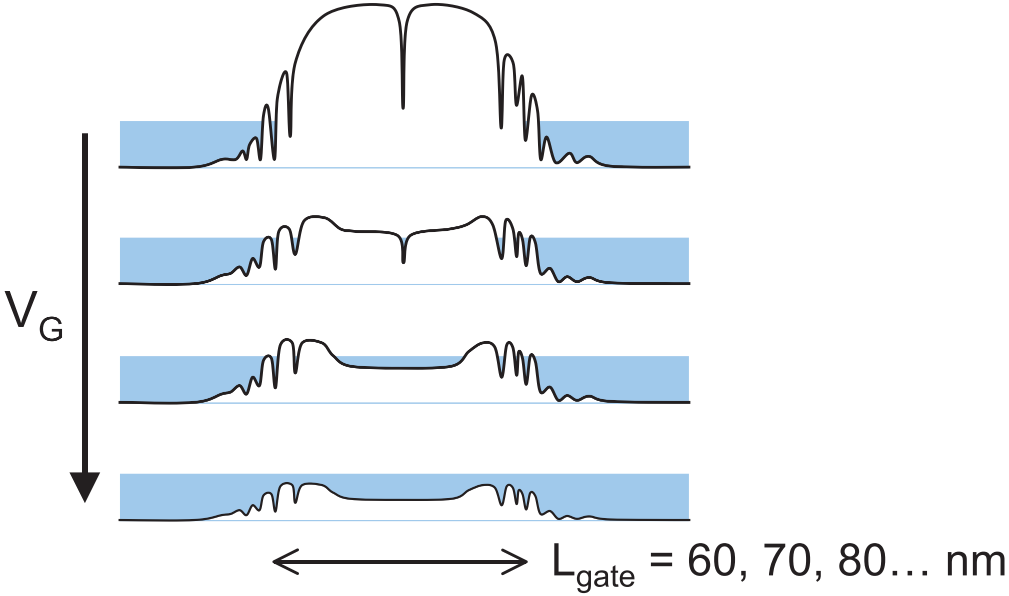
[Nadine Collaert, IMEC]

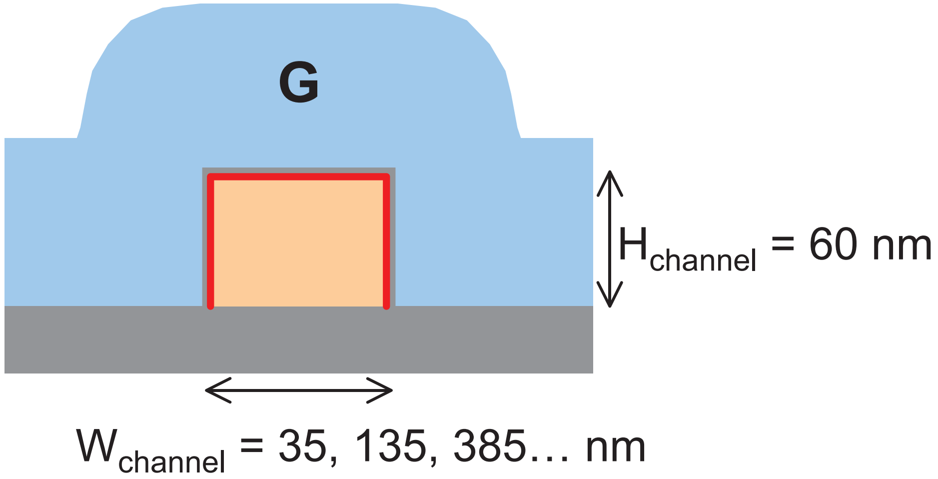
- application: lithographically defined Si nanowires (fins) covered by a single gate
- our experiments: single fin devices, here fin width 15 nm & gate length 20 nm

Transport through a FinFET

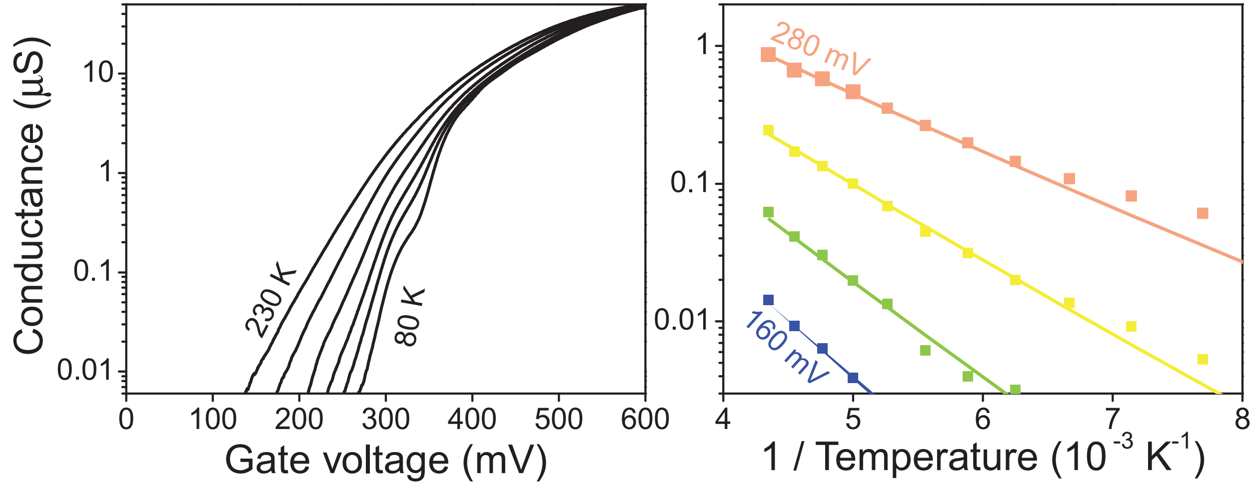


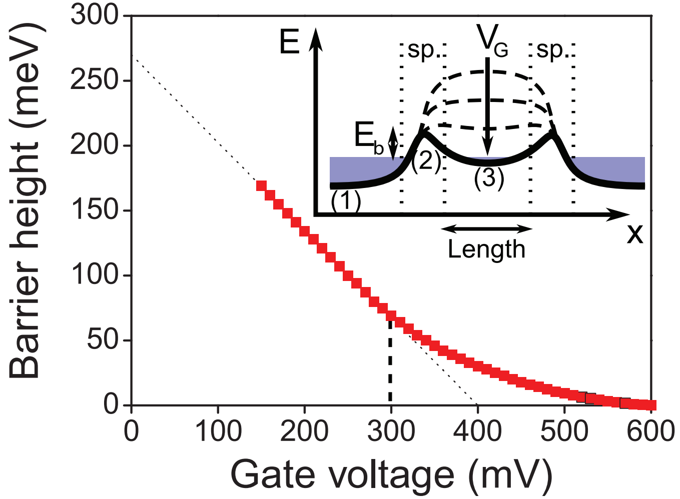






Thermionic emission in a FinFET: corner effect

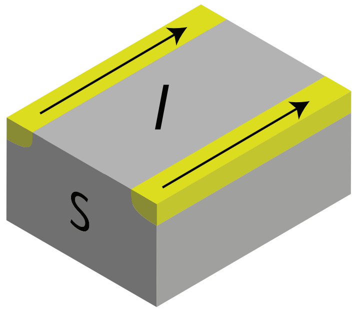




C

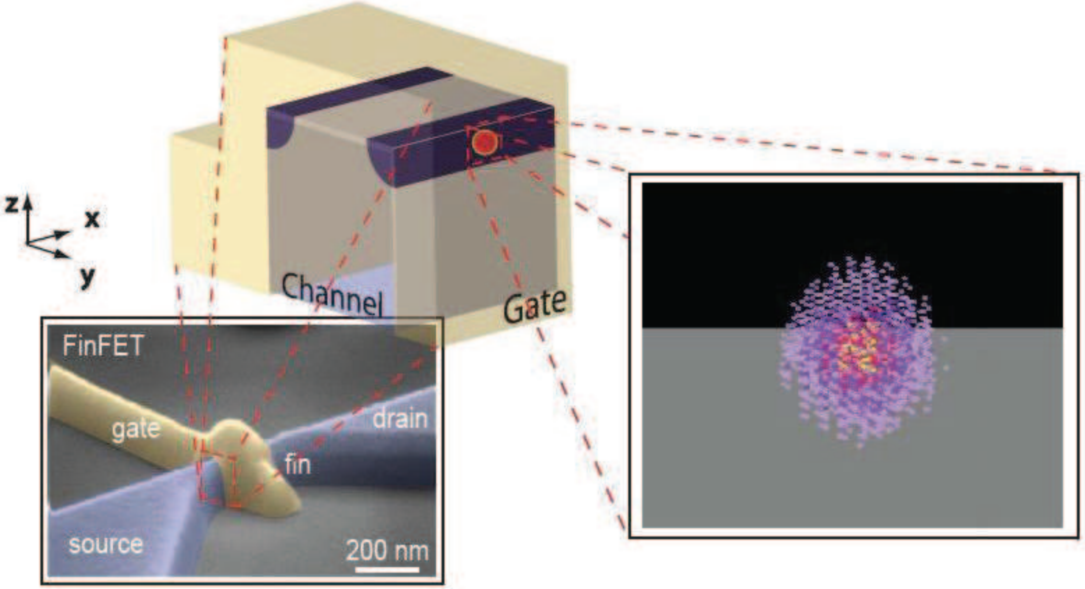
		L	
	S (nm²)	60 nm	120 nm
W	135 nm	**2.0**	**4.4**
	385 nm	**3.8**	**4.1**

[Sellier Appl. Phys. Lett. 90, 073502, 2007]

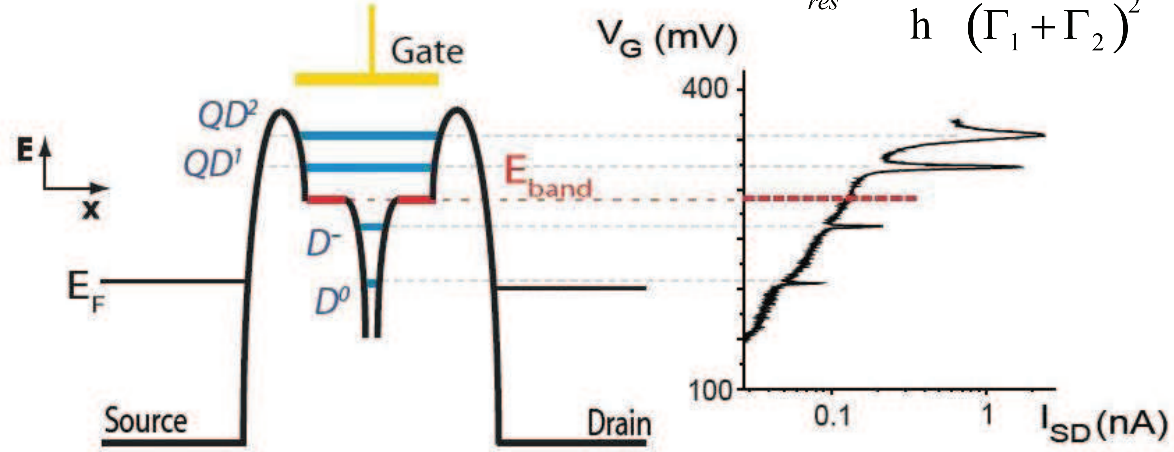


- $G = SA^*\frac{e}{k_\mathrm{B}}T\exp\left(-\frac{E_\mathrm{b}}{k_\mathrm{B}T}\right)$ [A^* for Si is 2.1×120 Acm^{-2}K^{-2}] $\Rightarrow$ S=4 nm^2
- strong coupling 0.67, decreasing gate action above 300 mV due to barriers

Resonant Tunneling Spectroscopy: States below the bandedge



$$G_{res} = \frac{4e^2}{h} \frac{\Gamma_1 \Gamma_2}{(\Gamma_1 + \Gamma_2)^2}$$



1 in 7 samples shows two peaks below the bandedge with lower conductance and larger peak separation

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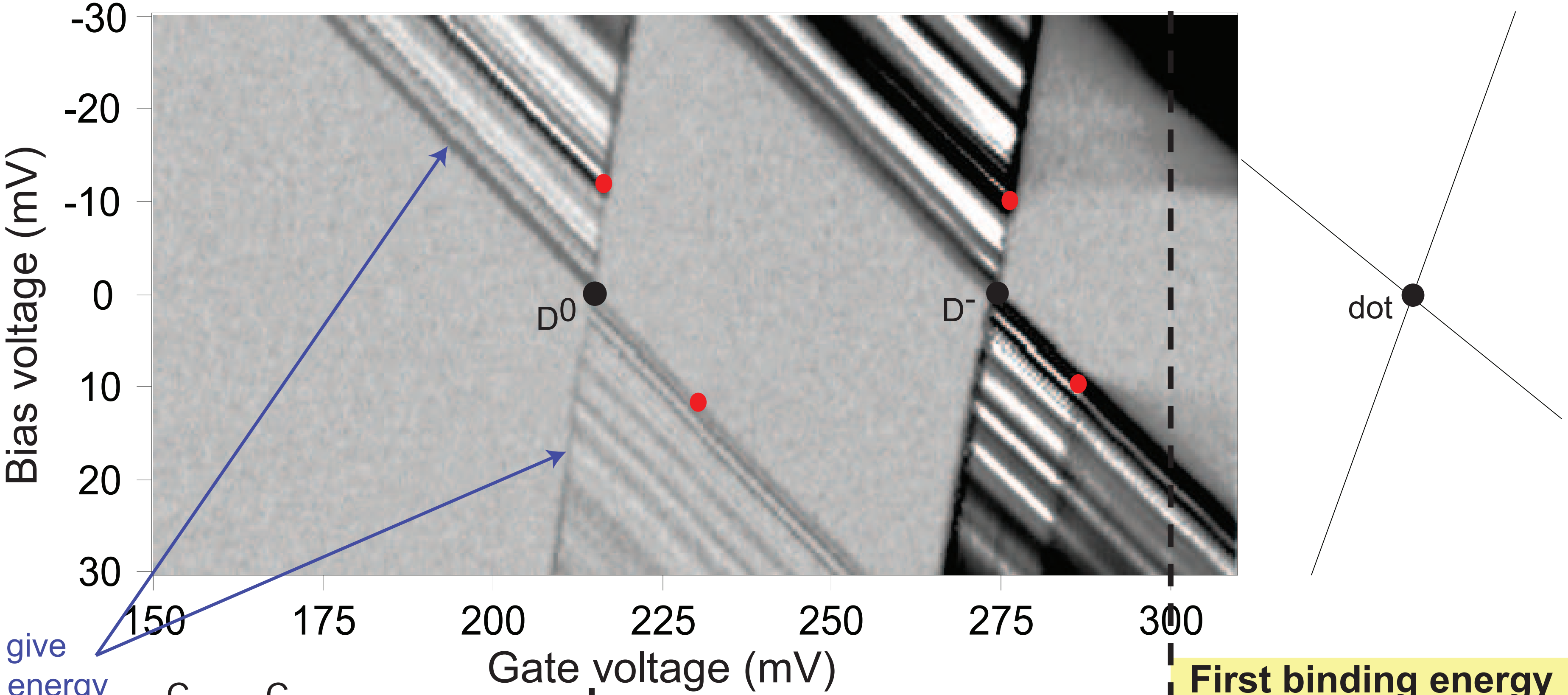
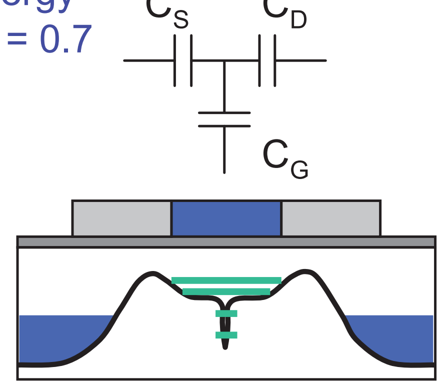
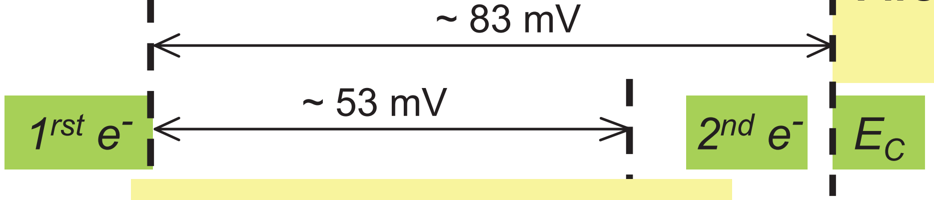
Stability diagram: the addition-spectrum



Slopes give voltage to energy conversion α = 0.7





Charging energy = 35 meV

First binding energy = 55 meV

⇓

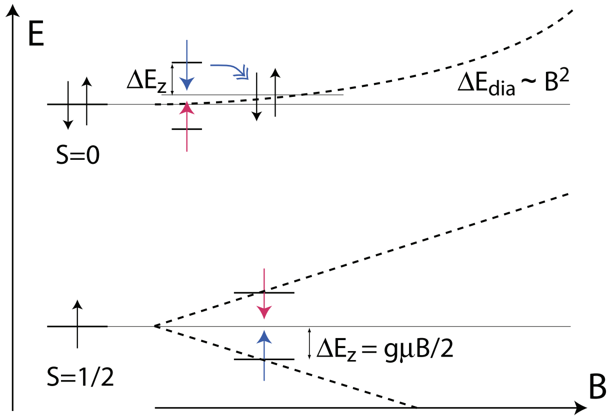
As: 54 meV
(P: 46 meV)

⇒ lower than 52 meV (As: 2 meV second binding energy)

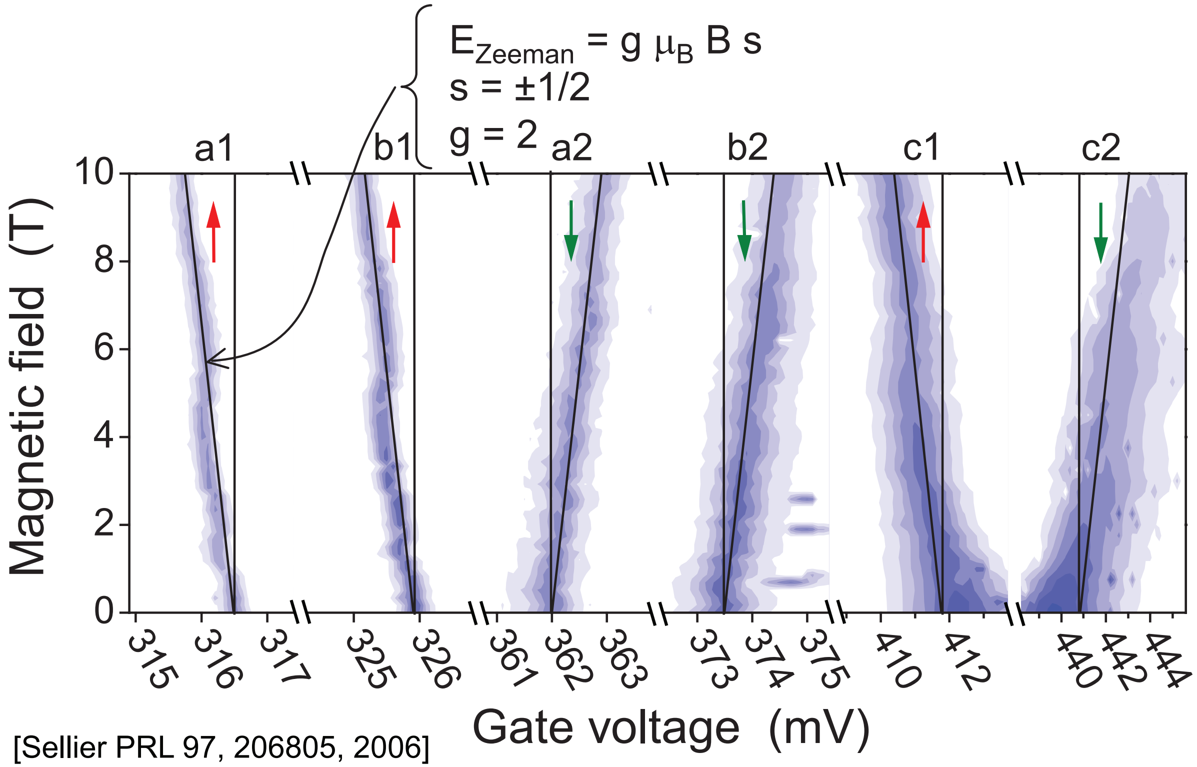
⇒ **increased capacitance** due to nearby electrodes

Magnetic Odd / Even effects in transport spectroscopy

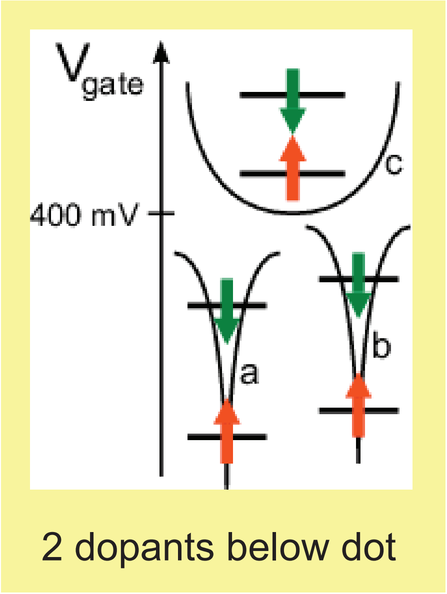
- first e^- → Zeeman shift *down*
- second e^- → Zeeman shift *up*
- singlet → spin selective formation!
- Zeeman shift with g=2
- independent of direction
  → no orbital effect ⇒ dopant



[theory by Engel PRB 65, 195321, '02]

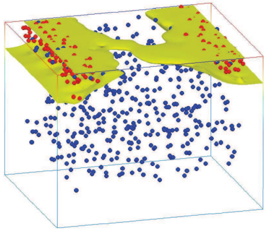


[Sellier PRL 97, 206805, 2006]

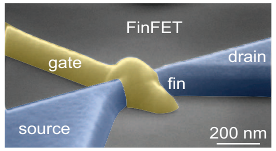


2 dopants below dot

Outline



- Atomic-scale electronics



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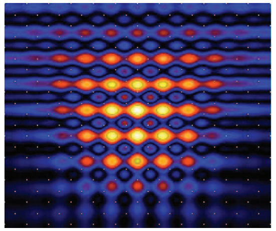
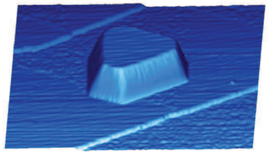


- Atomic physics in a MOSFET

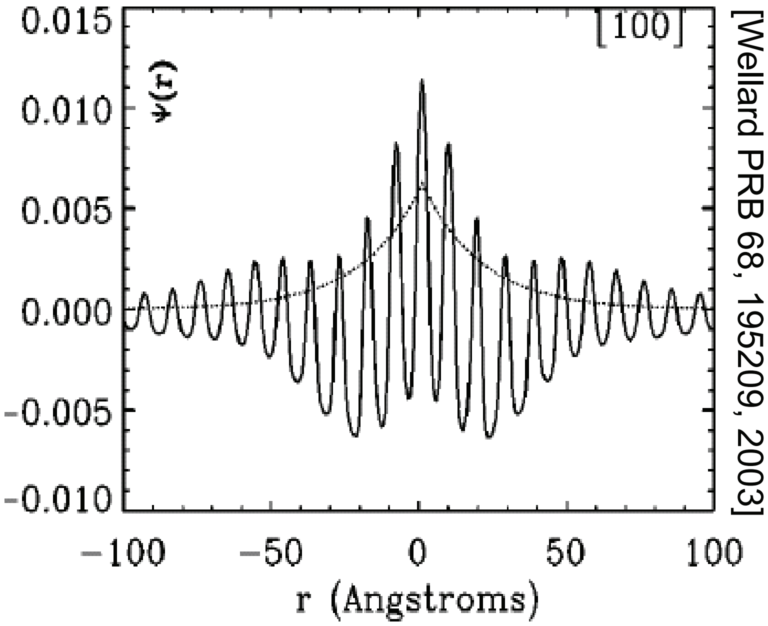
Σ

- Summary



- Other projects

Atomic physics in the solid state



[Wellard PRB 68, 195209, 2003]

Level	P	As
1s(A_1)	45.6	53.8
1s(T_2)	33.9	32.7
1s(E)	32.6	31.3
$2p_0$	11.5	11.5
$2p_{+/-}$	6.4	6.4
$3p_0$	5.5	5.5
$3d_0$	3.8	3.8

[Ramdas Rep. Prog. Phys. 44, 1981]

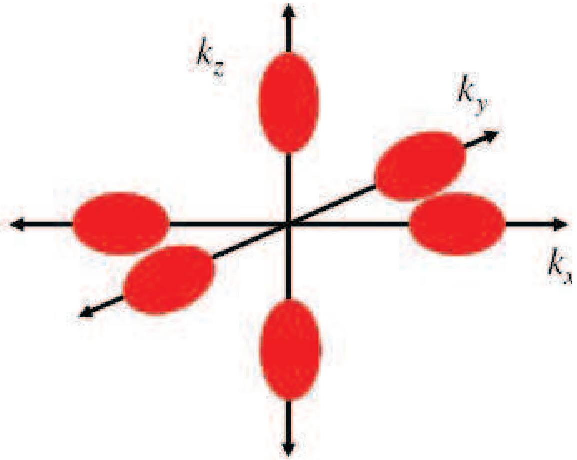
Kohn & Luttinger donor wavefunction in Si

$$\psi(\mathbf{r}) = \int F(\mathbf{k})\phi_{\mathbf{k}}(\mathbf{r})d\mathbf{k} \quad [H_0 + U(\mathbf{r})]\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

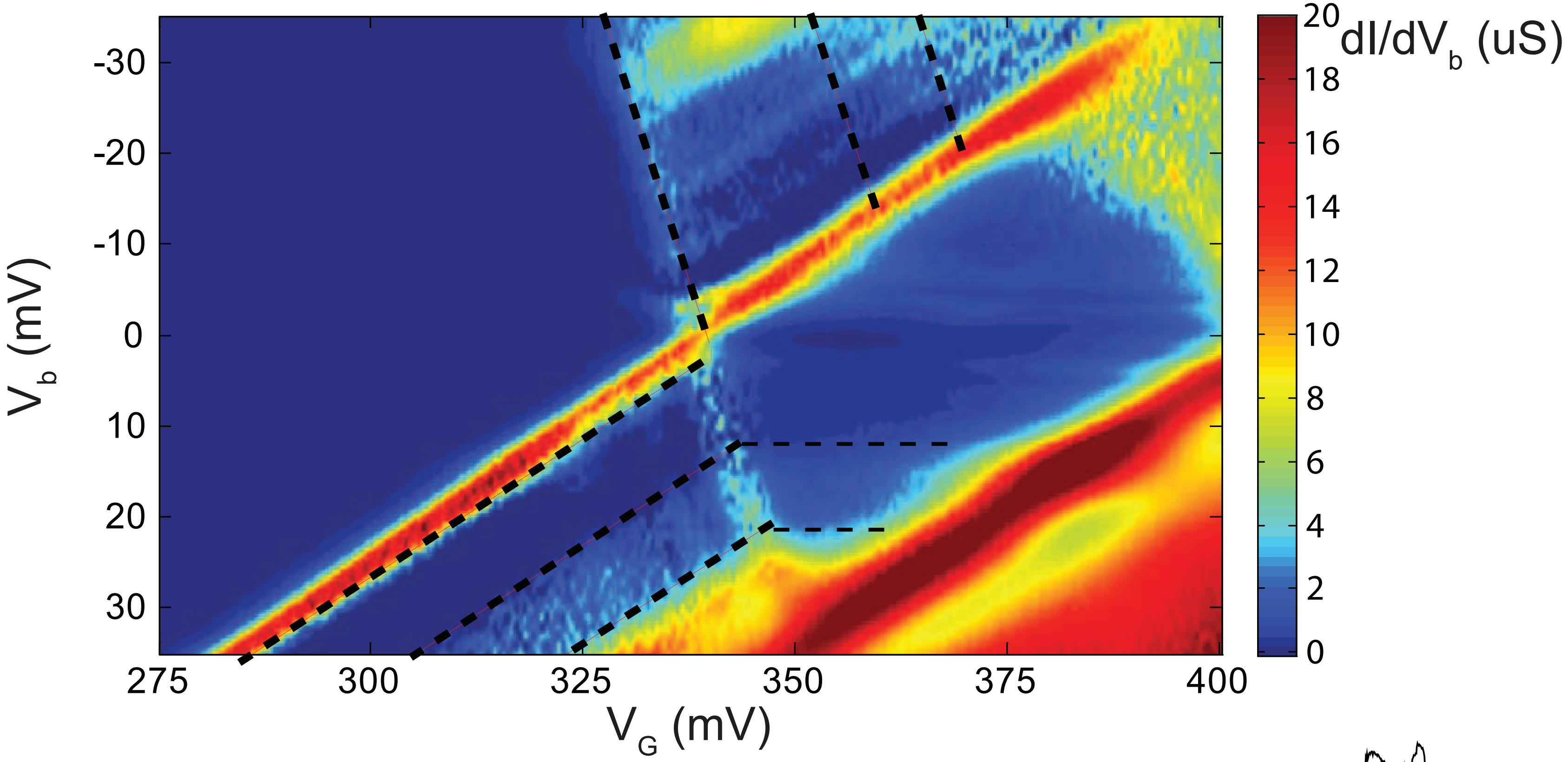
in basis of Si Bloch functions

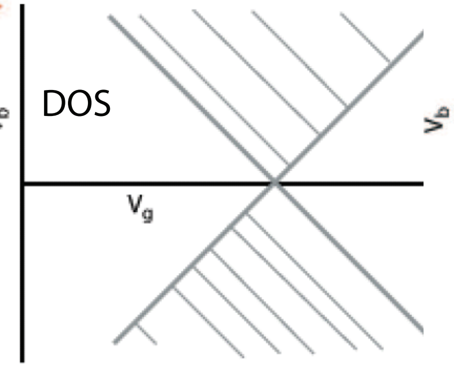
Properties of the envelop function:

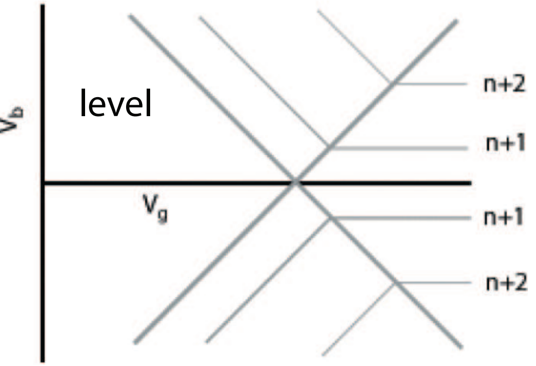
- non-degenerate ground state of A_1 symmetry
- excited triplet of symmetry T_2
- next, excited doublet of symmetry E

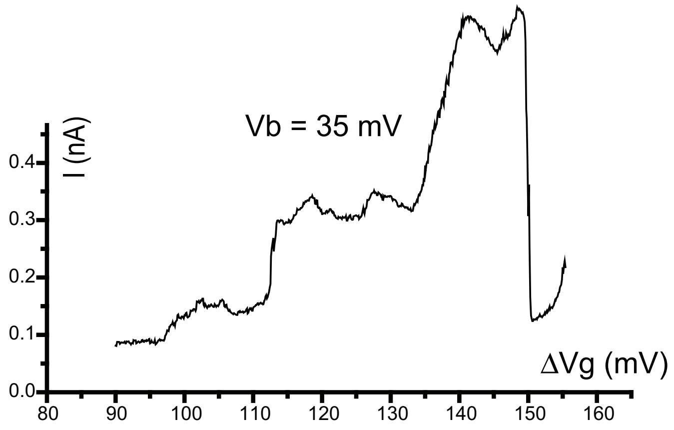


Assignment of the level spectrum

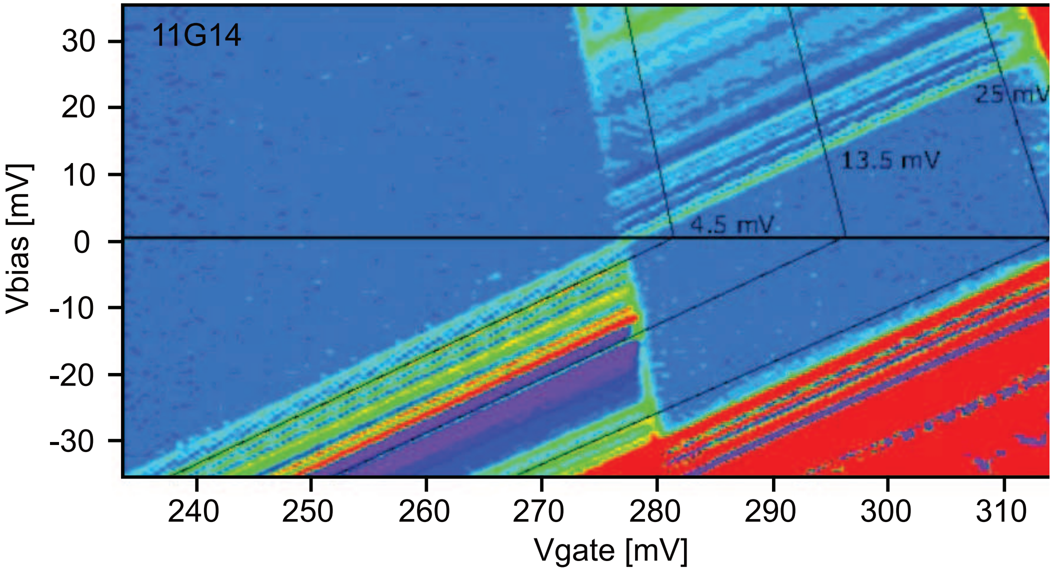


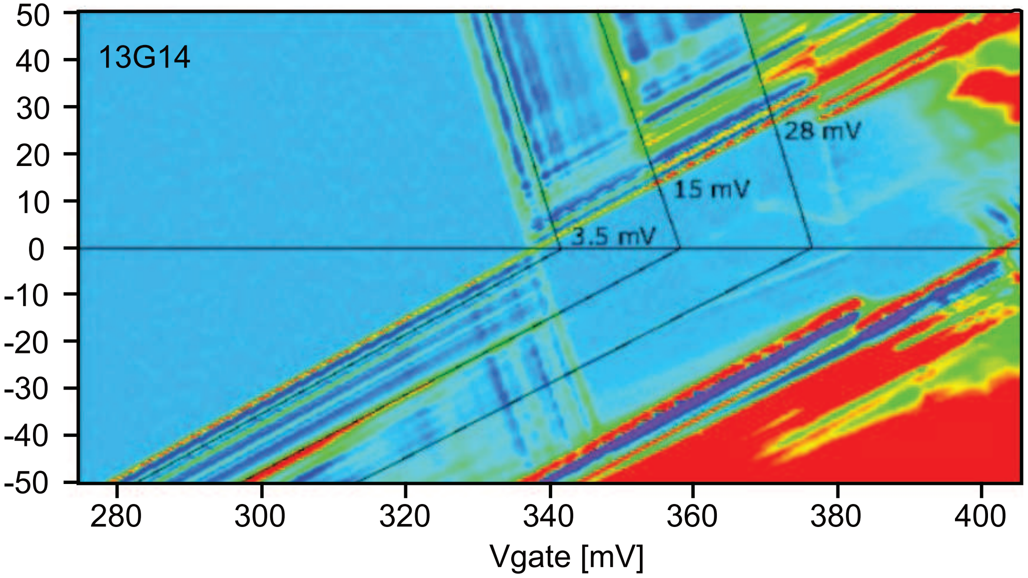


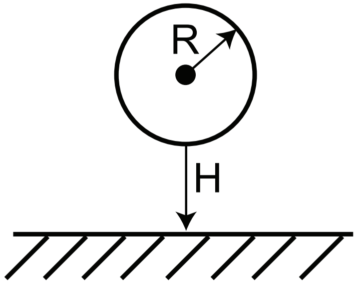




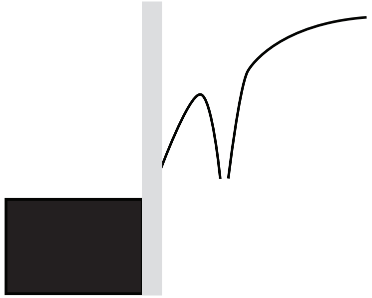
The environment of the dopant







Sample nr.	E_C (meV)	d (nm)
HSJ18	32	3.8
GLJ17	33	4.0
GLG14	35	4.7
13G14	29	3.2
11G14	29	3.2
10G14	30	3.3

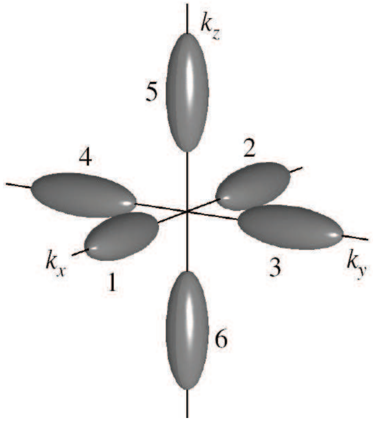


- *excited states spectrum* and *charging energy* differ from device to device
- use charging energy to determine dopant position based on capacitance
- dopant close to interface → region of strong band bending

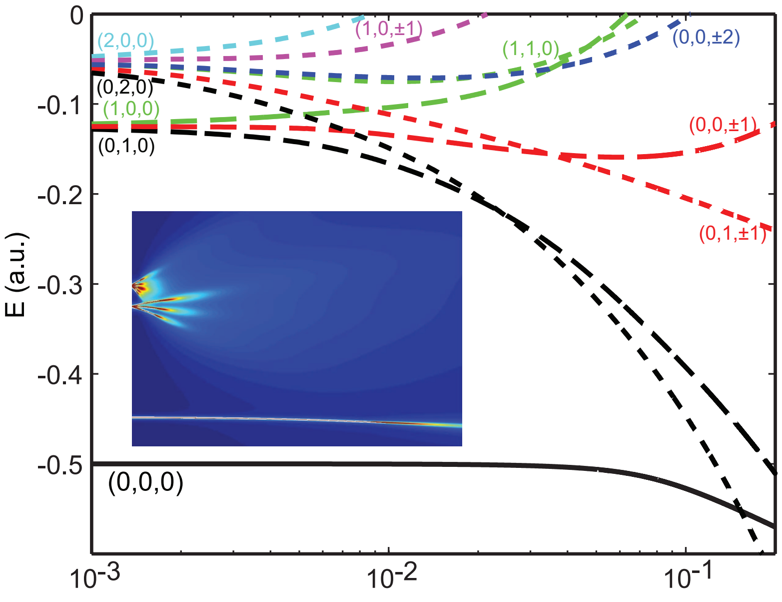
Effect of the electric field: Stark shift

Level	P	As
$1s(A_1)$	45.6	53.8
$1s(T_2)$	33.9	32.7
1s(E)	32.6	31.3
$2p_0$	11.5	11.5
$2p_{+/-}$	6.4	6.4
$3p_0$	5.5	5.5
$3d_0$	3.8	3.8

[Ramdas Rep. Prog. Phys. 44, 1981]

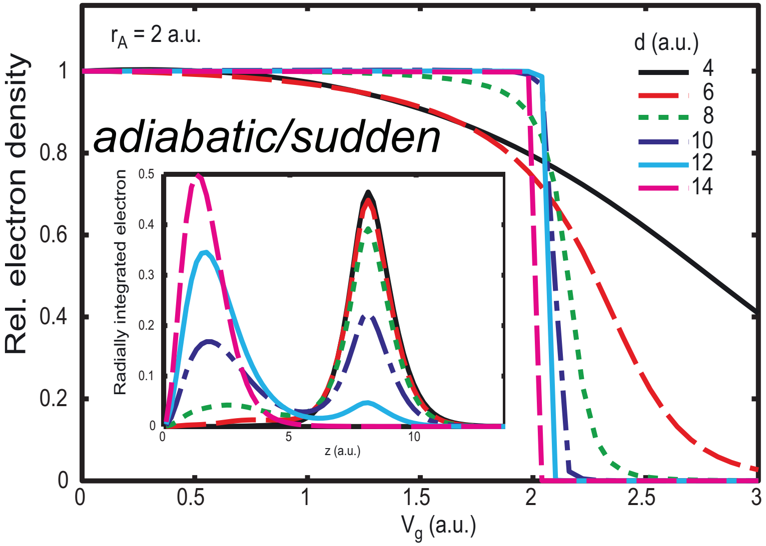


non-degenerate ground state, excited triplet,excited doublet



[Smit PRB 70, 035206, 2004]

Sample	1^{st} E_{ex} (meV)	2^{nd} E_{ex} (meV)	3^{rd} E_{ex} (meV)
10G16	2	23	>23
11G14	4.5	13.5	25
13G14	3.5	15	28
HSJ18	4.5	15.5	25.5
GLG14	1.5	10	25
GLJ17	7.5	15	22.5

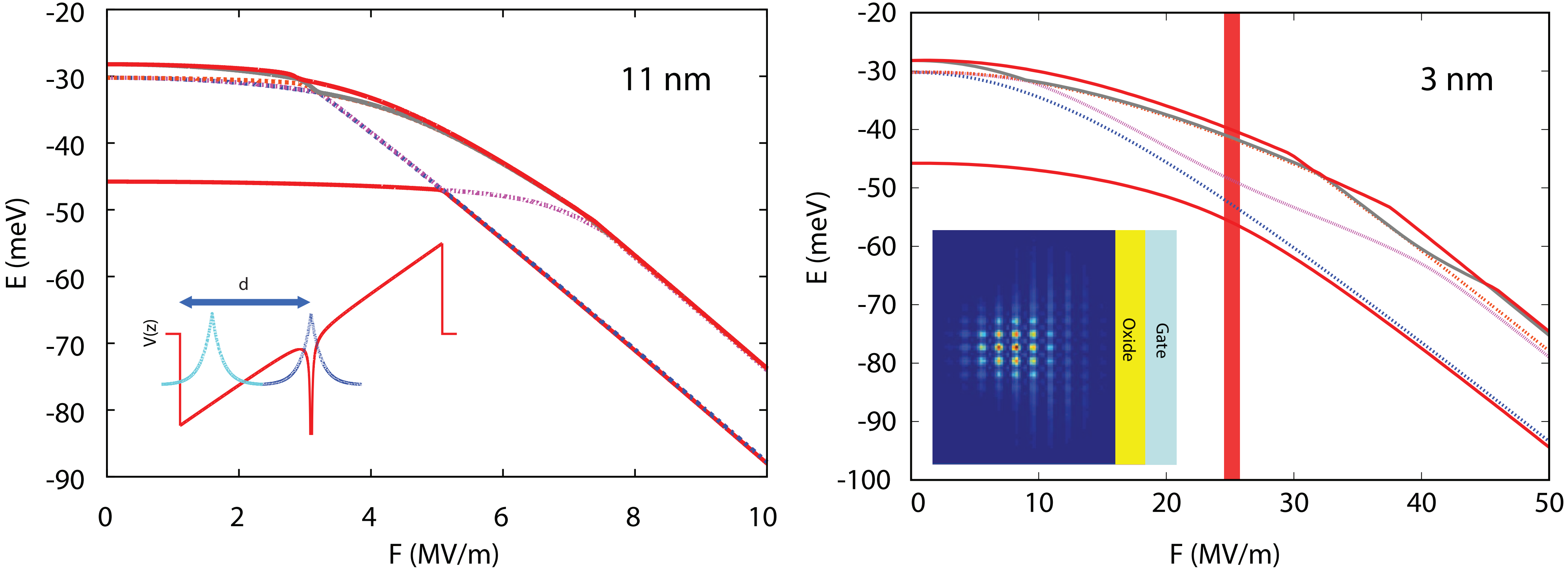


[Smit PRB 68, 193302, 2003]

similar work by: Martins, PRB 69, 085320, 2004; Friesen PRL 94, 186403 2005; Debernardi, PRB 74, 035202, 2006

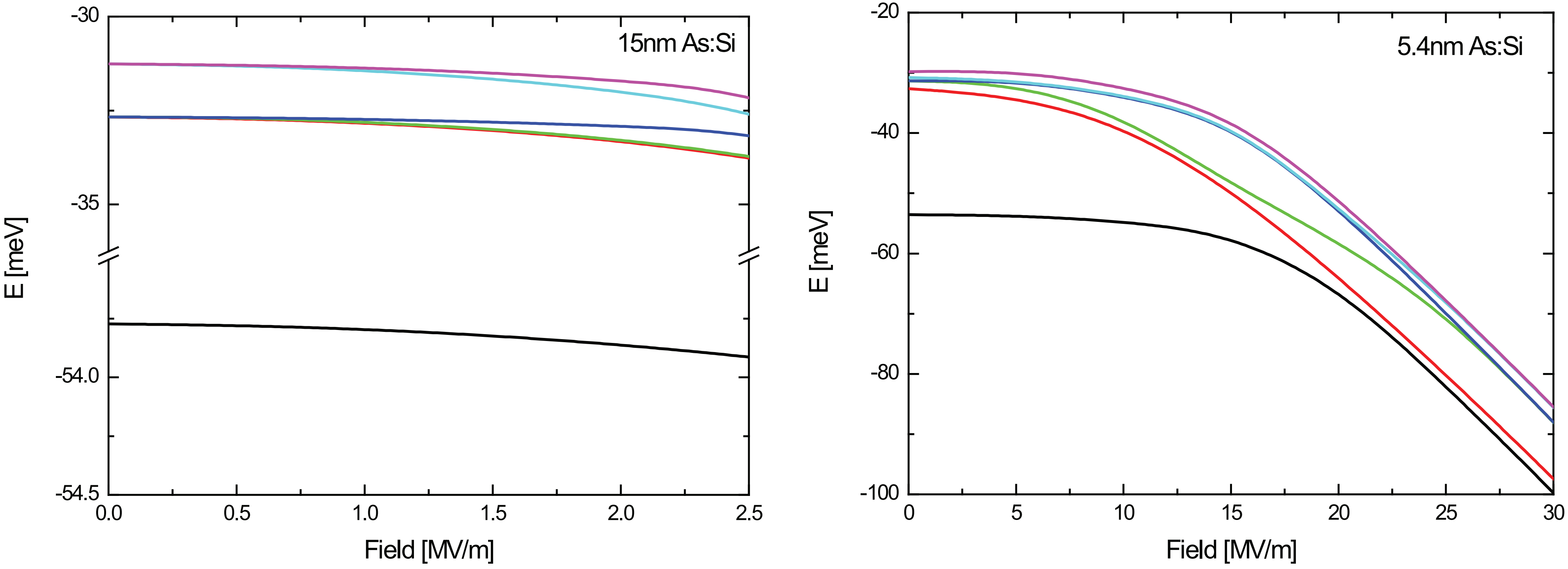
Calculation of donor/well system for P:Si

numerical diagonalization of the Hamiltonian in a band minima basis by our collaborators
Cam Wellard & Lloyd Hollenberg, Melbourne University



- below 5 nm donor/interface distance hybridization leads to avoided crossings
- hybrid wavefunction has a strong contribution of the dopant

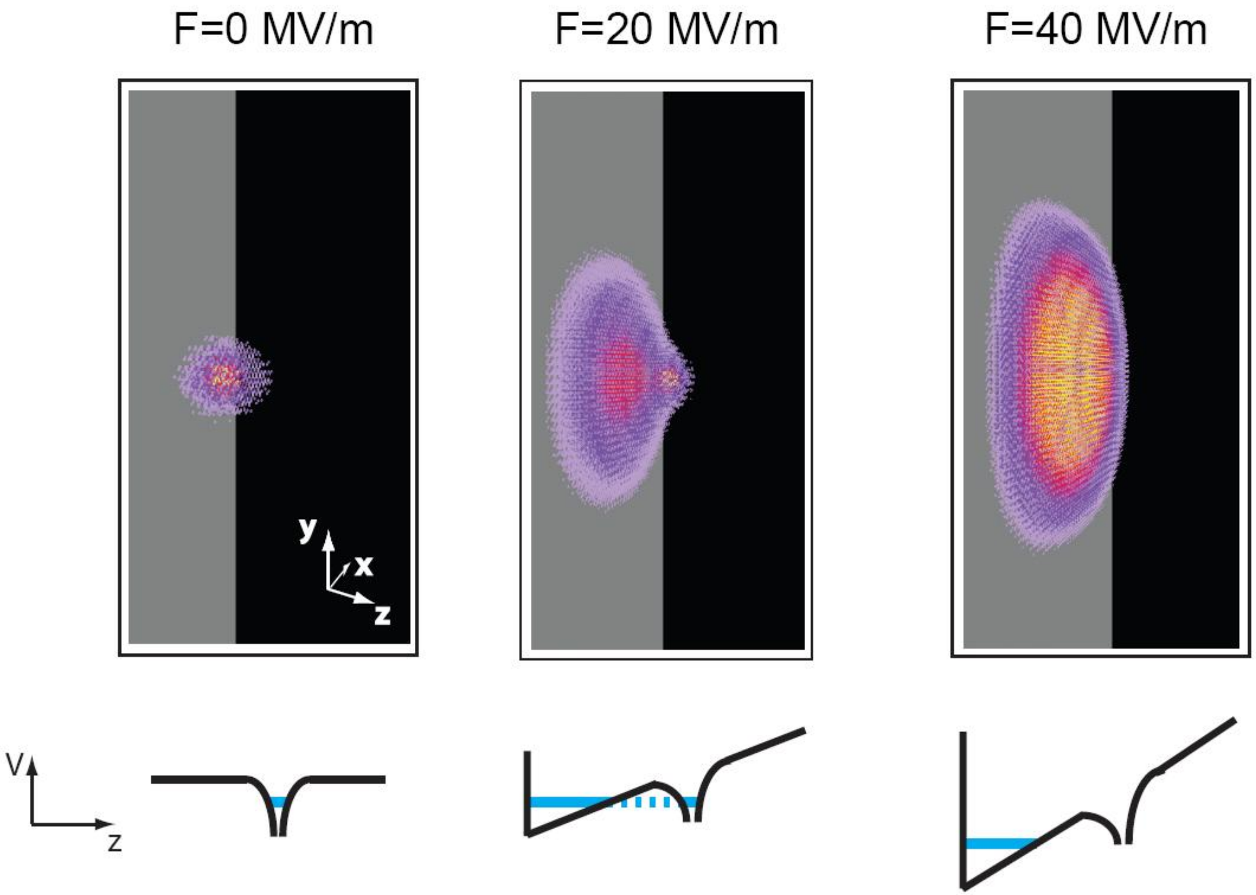
NEMO for our situation: Arsenic donor 3-6 nm from the interface

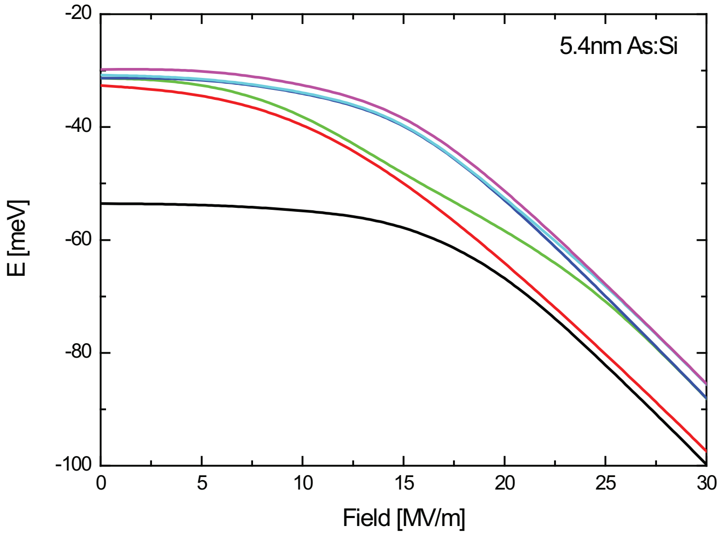


- perfect agreement of the tight binding calculation with bulk measurements
- a dopant close to interface leads to an anti-crossing region

[NEMO work by Rajib Rahman in Gerhard Klimeck's group at Purdue together with Hollenberg]

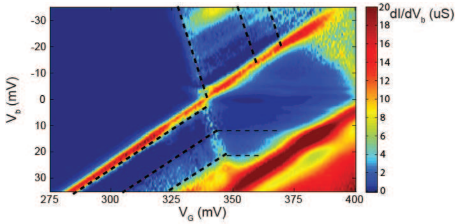
Hybridization with well state leads to a molecular system





co.: Rajib Rahman & Gerhard Klimeck (Purdue) and Cam Wellard & Lloyd Hollenberg (Melbourne Uni.)

Fit excited states of the dopants to model



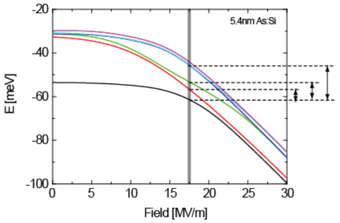
Measured

$E_{x,i}$

F ? , d ?

Predicted

$E_{x,i}$ **(F,d)**

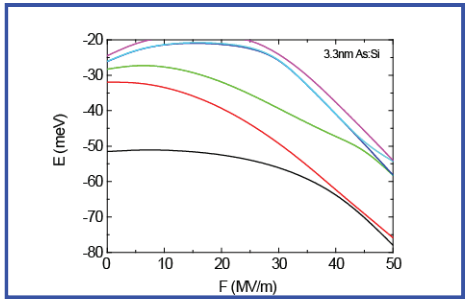


Sample	10G16	11G14	13G14	HSJ18	GLG14	GLJ17
Measured Ex1 (meV)	2	4,5	3,5	5	1,3	2
Measured Ex2 (meV)	15	13,5	15,5	10	10	7,7
Measured Ex3 (meV)	23	25	26,4	21,5	13,2*	15
Predicted F (MV/m)	37,3	31,6	35,4	26,1	23,1	21,8
Predicted r (nm)	3,34	3,51	3,24	4,05	5,16	4,92
Chi-square	0,59	0,04	0,17	0,63	0,28	0,96
Ex1 (meV)	2,2	4,5	3,6	4,9	1,8	1,1
Ex2 (meV)	15,6	13,5	15,7	10,2	10,0	7,7
Ex3 (meV)	23,0	25,0	26,3	21,4	13,2	15,3

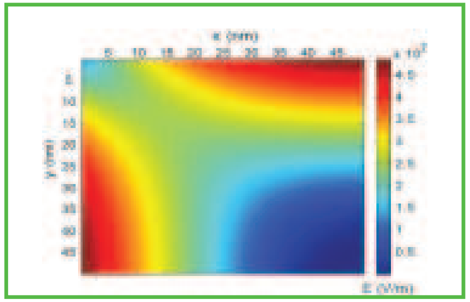
- a 2D (F, d) fit of the first 3 excited states of the model works well for the 6 samples
- S_{total}(As)=0.53 meV equal to the measurement error
- S_{total}(P)=1.5 meV leading to a 0.99 certainty for the As model

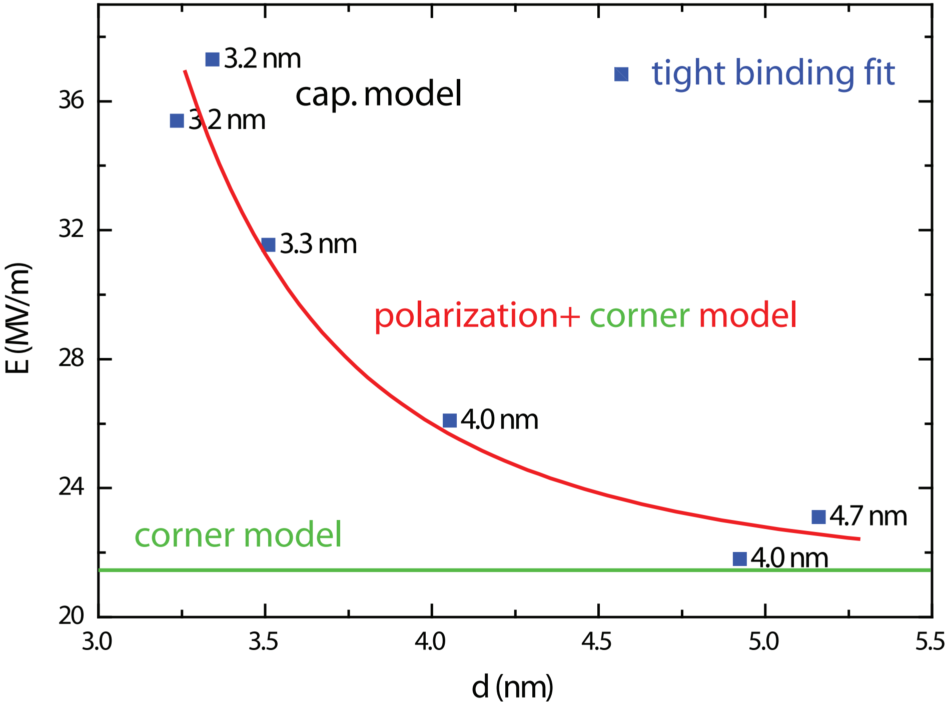
Comparison between data and model in a broader context

Tight binding

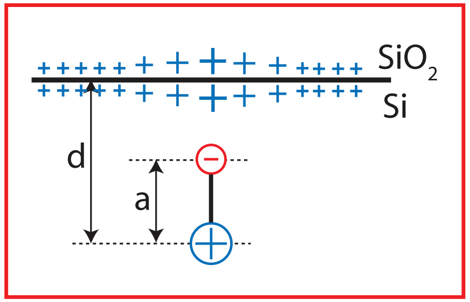


Corner effect

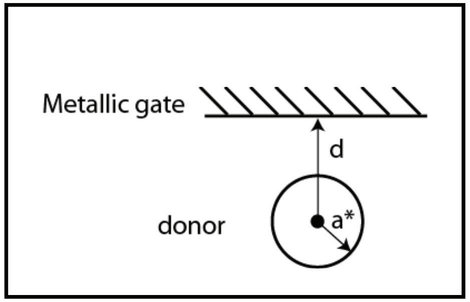




Polarization



Capacitive model



- field at the dopant site is higher than expected from the corner model
- magnitude and functional form of polarization layer + corner field fit well
- independent capacitive data in decent agreement with tight-binding fit

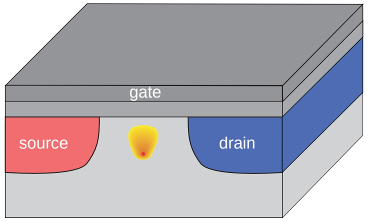
[paper in preparation by Delft, Melbourne, Purdue groups]

Summary

- Transport through a triple-gate nano-MOSFET
  - corner effect → 1D channel with $4\,\mathrm{nm}^2$ cross section

- Access to a single dopant
  - ionization energy of 1st e^- consistent with As in Si
  - charging energy for 2nd e^- lowered due to electrodes

- Atomic physics in a MOSFET
  - large E-field → strong Stark effect → new level spectrum
  - hybrid wavefunction of dopant and interface well, anti-crossing



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People involved

- Delft
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    - Paul Rutten, Gabri Lansbergen, Hermann Sellier, *vacancy* (FinFET)
    - Jaap Caro & Huub Salemink (group Photronic Devices)
- IMEC
    - Nadine Collaert & Serge Biesemans (FinFET)
- University of Melbourne
    - Cam Wellard, Lloyd Hollenberg (Theory)
- Purdue
    - Rajib Rahman, Gerhard Klimeck (NEMO)


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