The importance of valley splitting in few-electron donor based quantum dots in silicon

Martin Fuechsle[1]

S. Mahapatra[1], B. Weber[1], W. Pok[1], H. Buech[1], M. Friesen[2], M. A. Eriksson[2] and M.Y. Simmons[1]

[1]*University of New South Wales, Sydney, NSW 2052, Australia*
[2]*University of Madison, Madison 57306, Wisconsin, USA*

QIST Workshop

Berkeley, August 2008

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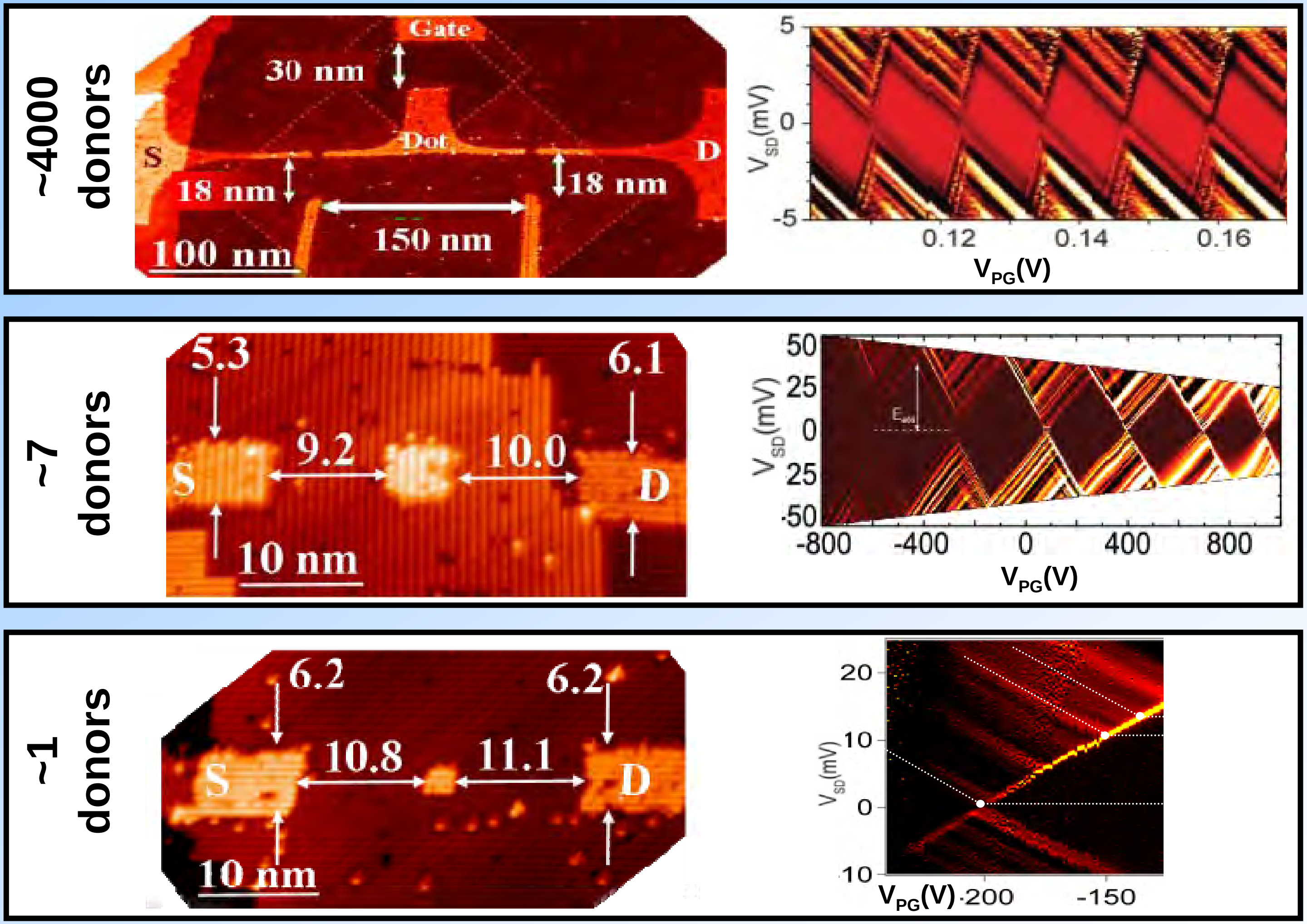
Atomically precise Si:P devices

- STM allows for atomically precise patterning of donor structures
- Goal: down-scaling to a single P donor

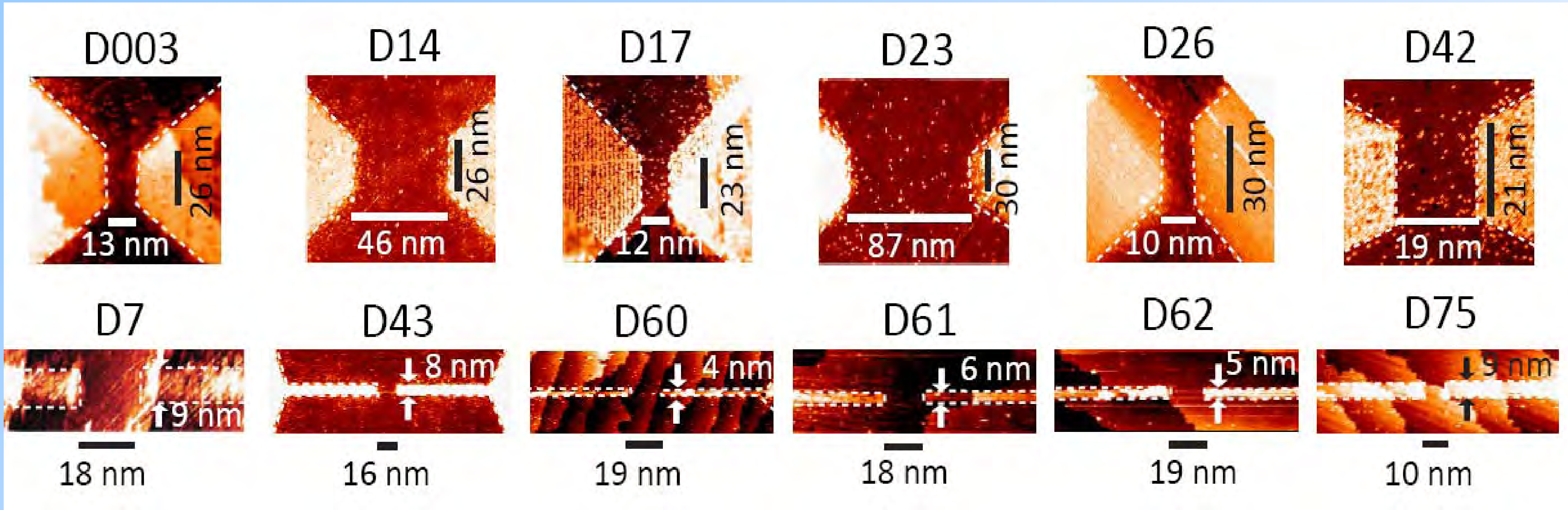
- Decreased number of donors from 4000 to the single donor limit
- ~7 donor quantum dot: surprisingly dense excitation spectrum observed → can be explained by valley splitting
- Effective mass calculations: valley splitting of dot states
- Single donor limit: evidence for excited states of a single P in Si
- Strategies for charge sensing

STM-patterned Si:P donor based quantum dots



A. Fuhrer, *et al., Nano Lett.* **9**, 707 (2009)

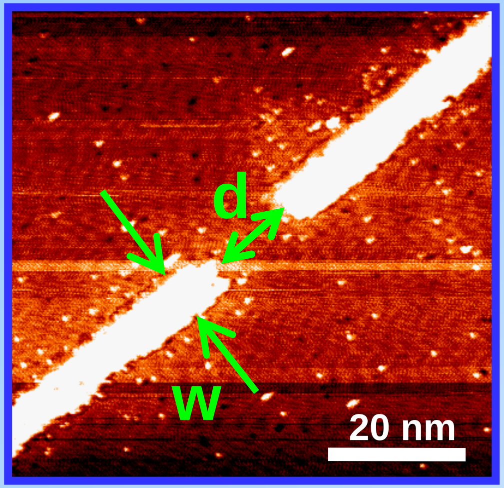
Tailoring the tunneling resistance



- Increased device yield now allows statistical study of device behaviour
- We fabricated a series of tunnel gaps to determine the effect of the gap geometry on the tunnel resistance

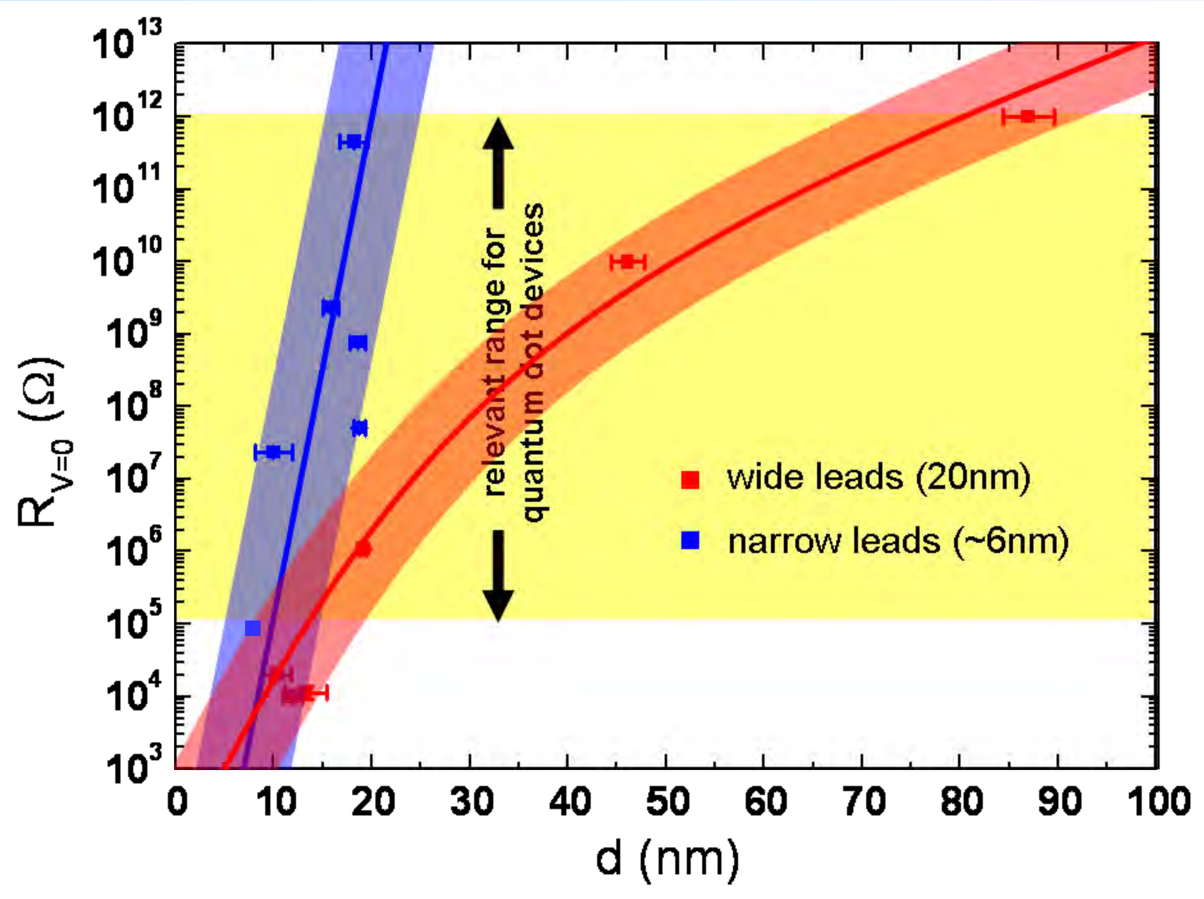
Tailoring the tunneling resistance

tunnel gap device



d = separation

w = lead width

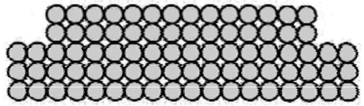


- Gap aspect ratio (w/d) determines transport characteristics
- These results allow us to predict device behaviour and improve device design

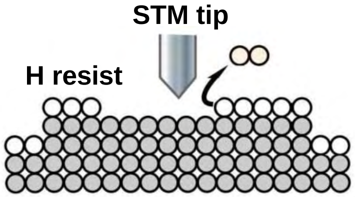
STM based fabrication

UHV

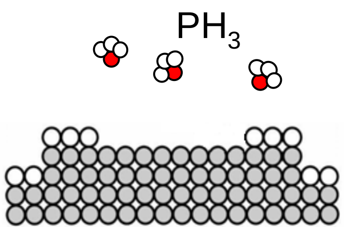
Step-free Si(100) surface



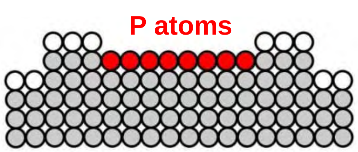
Initial anneal at 1100ºC



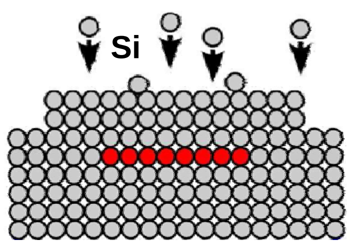
Use STM tip to desorb hydrogen



PH_3 adsorbs onto exposed Si



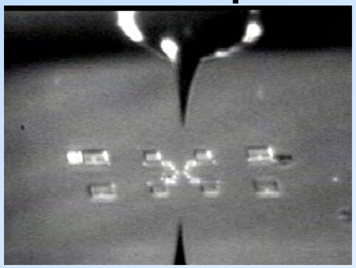
Incorporate P donors



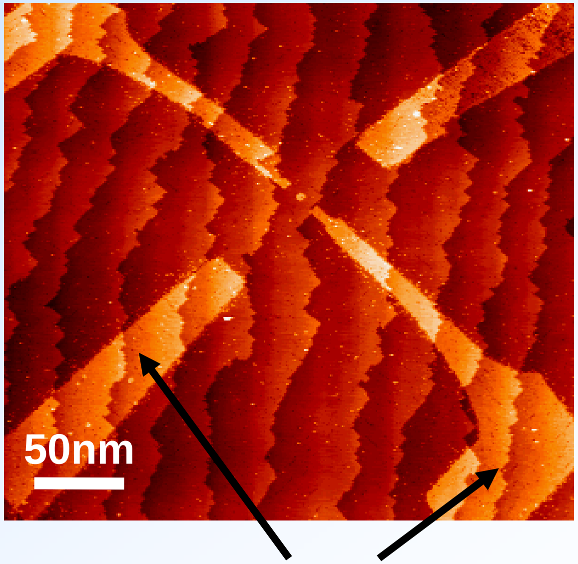
Encapsulation with 25nm of epitaxial Si

ex-situ processing: ohmic contacts and top-gates

STM tip

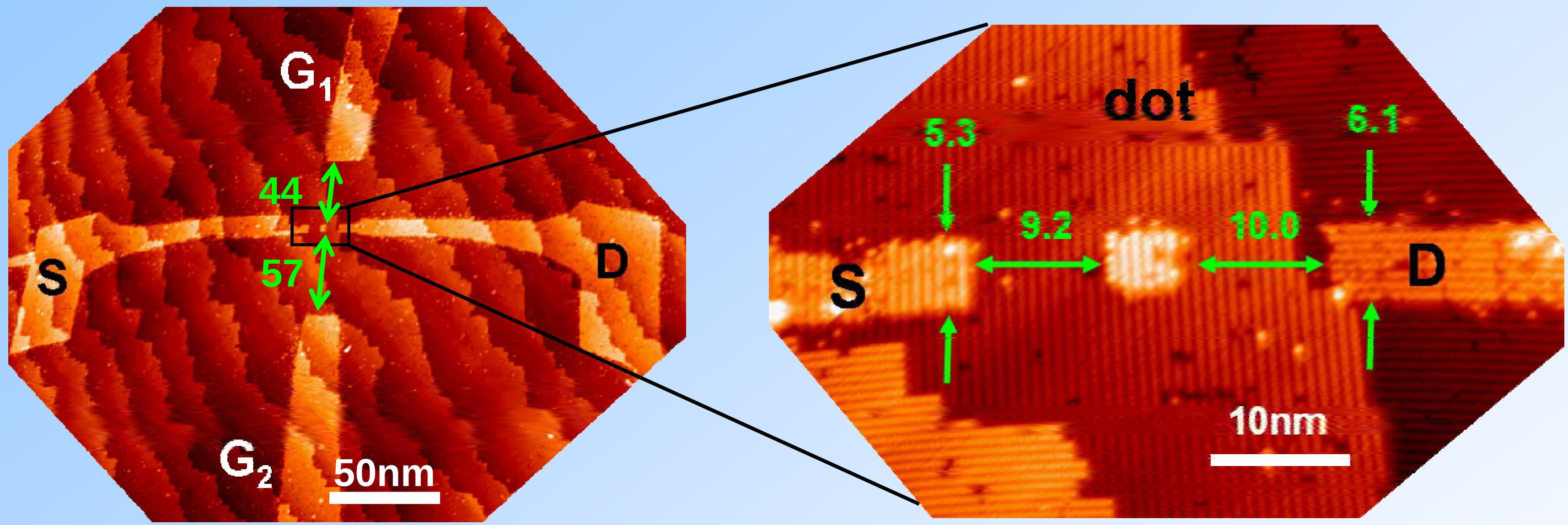


STM image of a quantum dot device



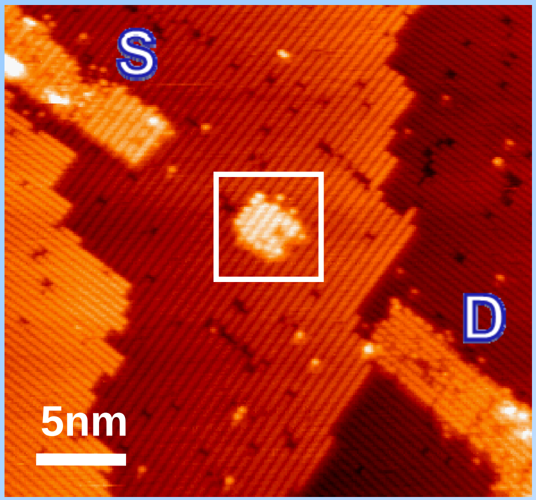
H desorbed regions appear brighter

Single crystal few-electron quantum dot

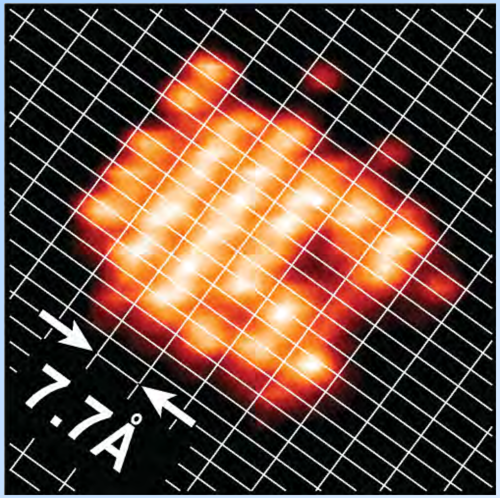


- 4 terminal quantum dot (4.6 x 4.6nm²)
- S,D leads, quantum dot, and gates are planar, highly P doped silicon
- Fully epitaxial structure, avoiding interface and surface related challenges

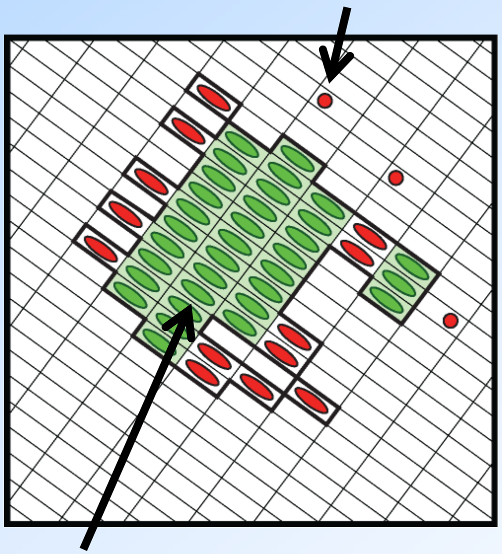
Accurate estimation of the number of donors



H lithography mask on Si(001)



Overlay grid with dimer row spacing

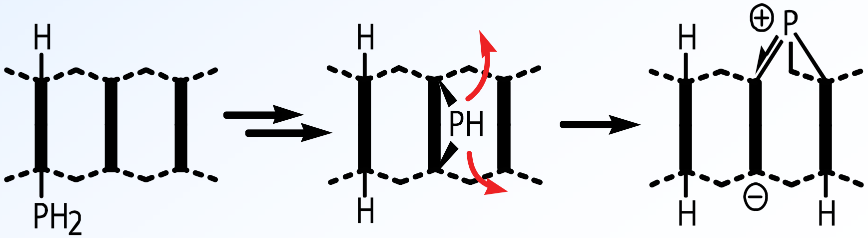


Possible P incorporation sites

- STM allows for direct counting of H-desorbed Si dimers/adsorption sites
- Detailed P incorporation mechanism previously studied*:

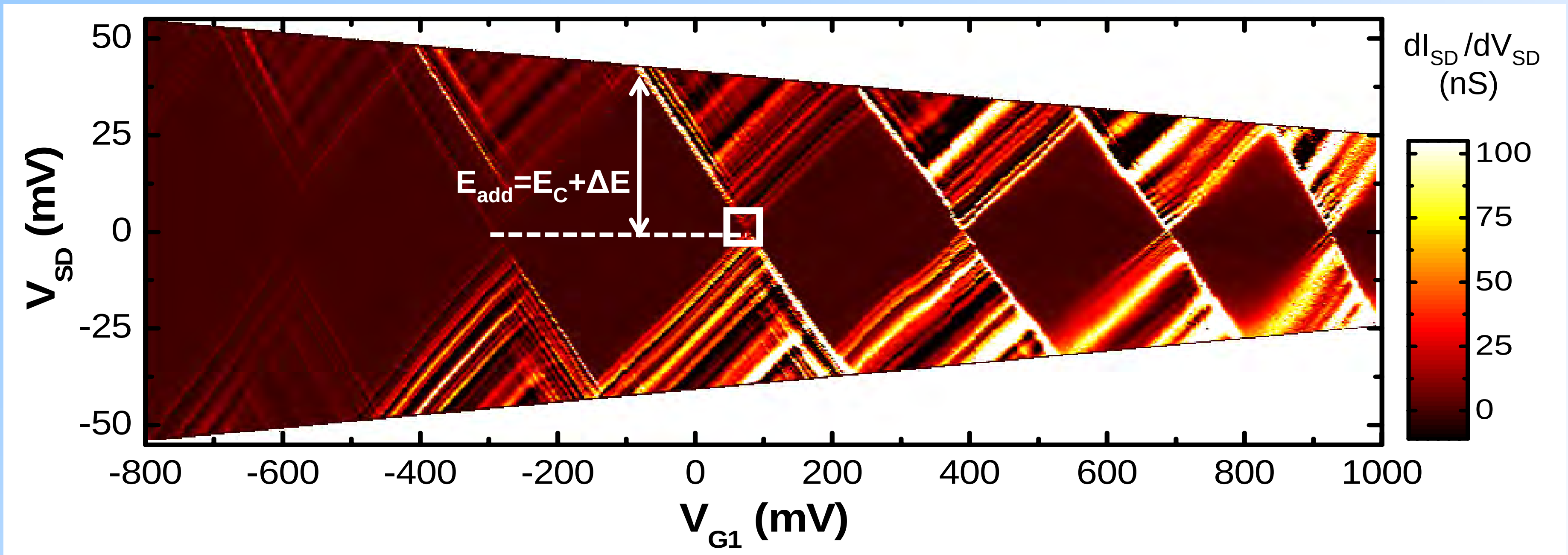
→ 3 adjacent dimers are required for 1 P atom to incorporate

- Statistical incorporation study for similar dot sizes ➔ **7 donors** most likely



* S. R. Schofield, *et al.*, *Phys. Rev. Lett.* **91** (2003)
H. F. Wilson, *et al.*, *Phys. Rev. Lett.* **93** (2004)
O. Warschkow, *et al.*, *Phys. Rev. B* **72** (2005)

Stability Plot at mK temperatures



• Gate voltage dependence of tunnel barriers:

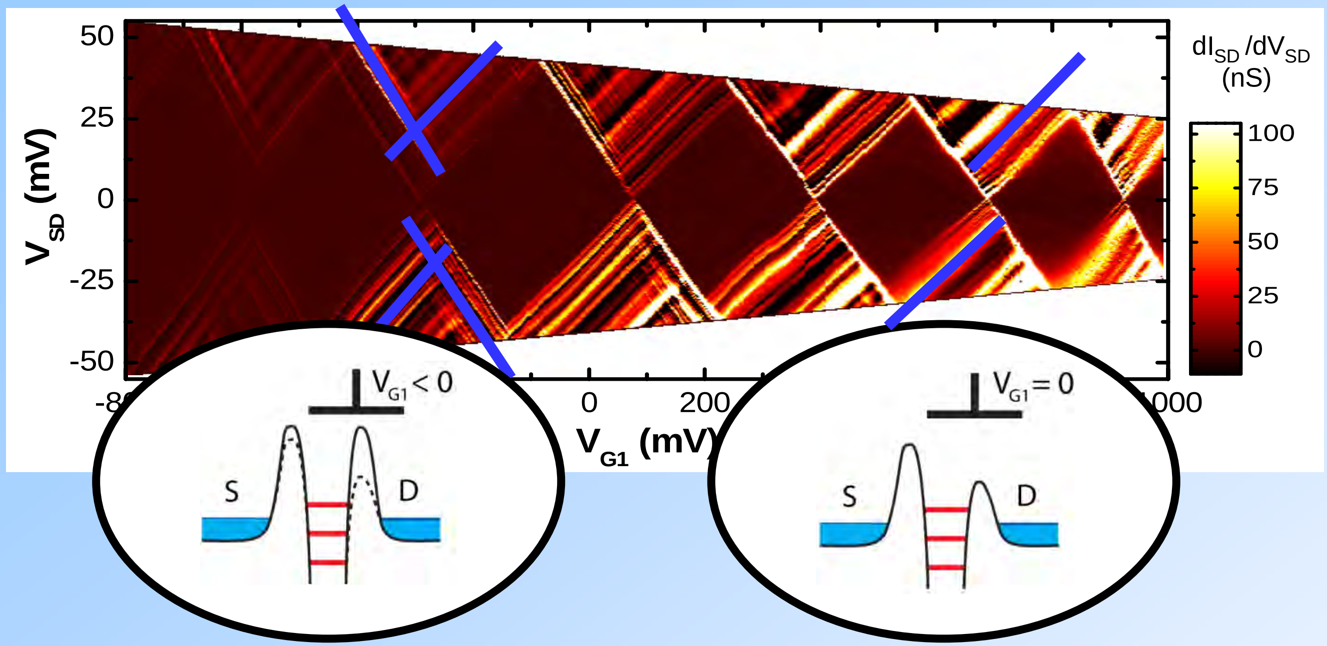
→ Increase in device conductance → change in coupling asymmetry

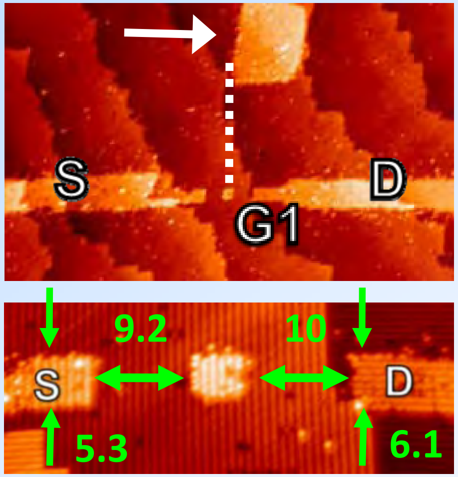
• Rise in addition energy as electron occupation is lowered → few-electron dot

• Surprisingly high density of lines of increased conductance

• Charge offset stability: < 0.01e over two days (within 30mV gate window)

Control of dot barrier asymmetry



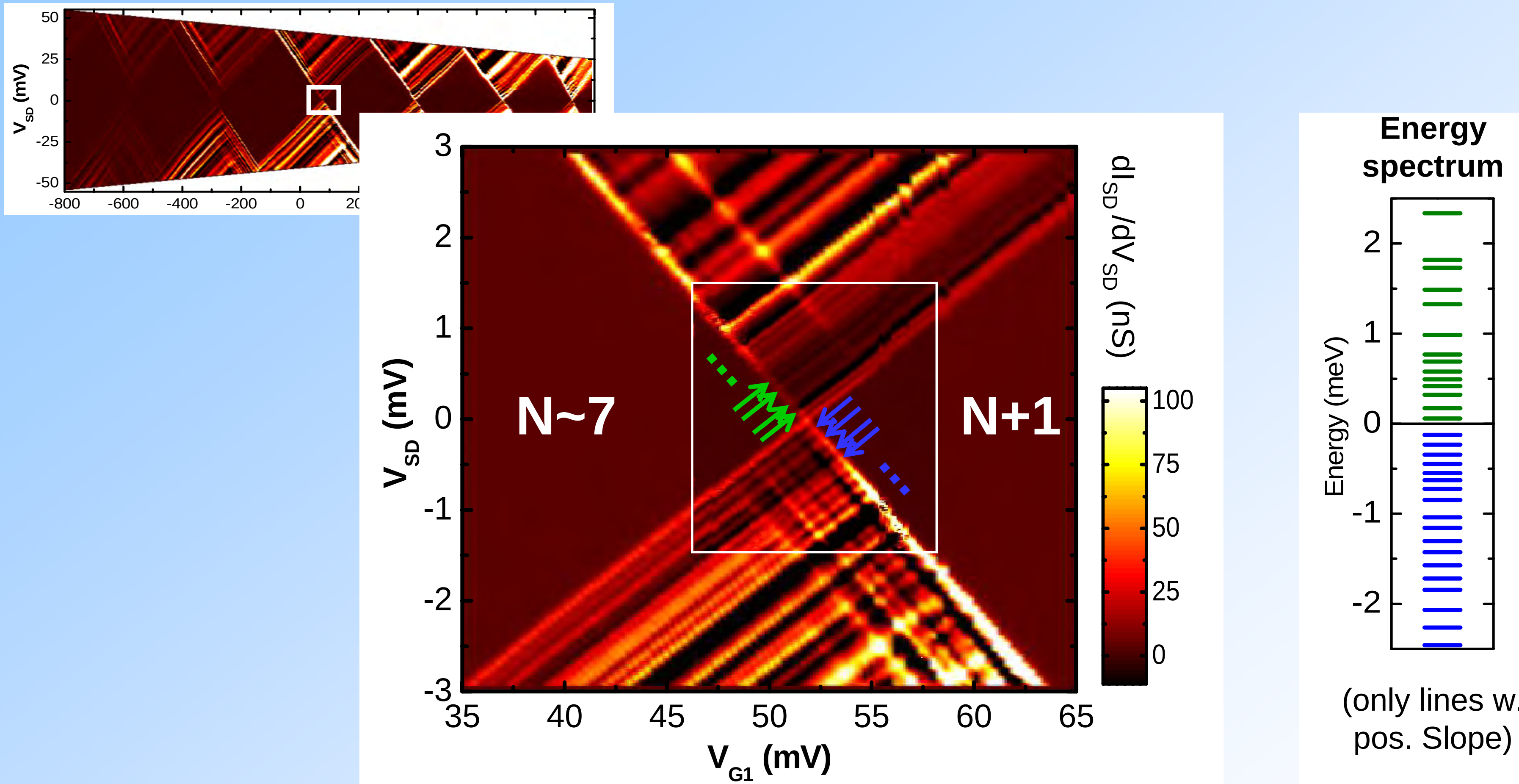


- $V_{G1} > 0$: we predominantly observe lines with positive slope

  → stronger *tunnel coupling* to D (higher gap aspect ratio: 0.61 > 0.58)

- Gate G1 shifted towards D: coupling asymmetry changes with gate voltage

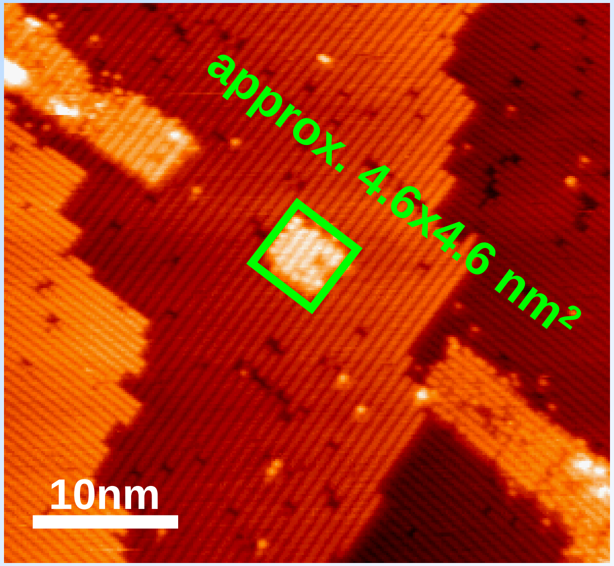
Surprisingly dense excitation spectrum



- Close-up of transition close to V_G=0 reveals even higher density of resonant features
- Average level spacing **ΔE ~ 130μeV**

➔ What is the origin of the resonant features?

Can these resonances be attributed to orbital excited states?



Estimate for the mean level spacing for laterally confined dots*:

$$\Delta E = \frac{\pi \hbar^2}{g m^* A}$$

→ Assume an effective mass $m^*_{ave} = 0.28\ m_e$

→ Assume max. degeneracy factor $g = g_{spin} \times g_{valley} = 2 \times 6$

$$\Delta E \sim 12\ \text{meV}$$

→ The tight lateral confinement cannot account for the dense excitation spectrum

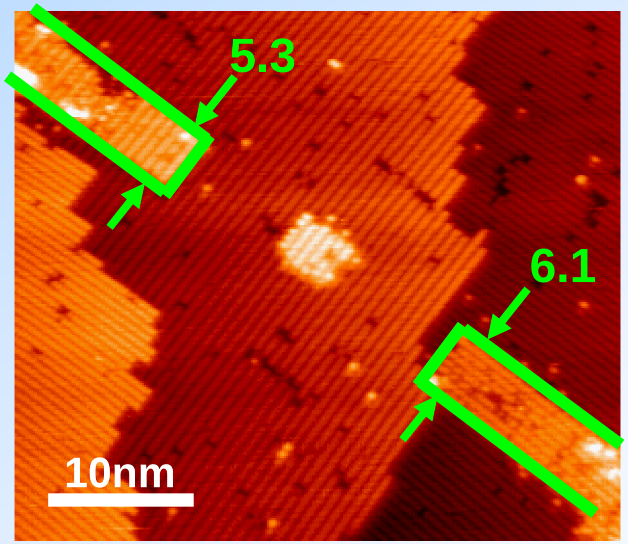
*L.P. Kouwenhoven *et al.*, *NATO Advanced Study Inst. on Mesos. Electron. Transp.* (1997)

[$m^*_{ave} = 0.28\ m_e$ from G. Qian, *et al.*, *Phys. Rev. B* **71**, 045309 (2005)]

Can they be density-of-states fluctuations in the leads?

- Quasi 1D transport in narrow (~6nm) S,D leads

→ Spacing of 1D subbands (for harmonic confinement)



$$\Delta E_n = \frac{\hbar\omega_0}{g} = \frac{\hbar}{g}\sqrt{\frac{8V}{m^* l^2}}$$

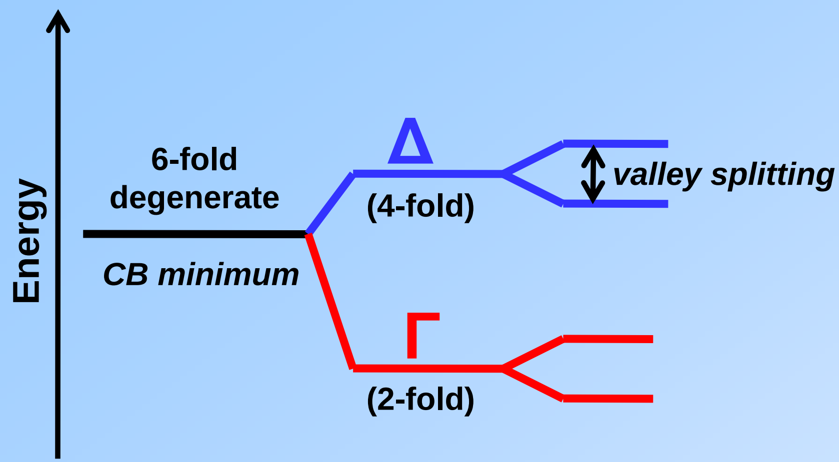
→ Assume g=12 and $m^*=0.28m_e$

→ Assume barrier height V=100meV (from detailed tunnel gap studies)

$$\Rightarrow \quad \Delta E_n \approx 7 \text{ meV}$$

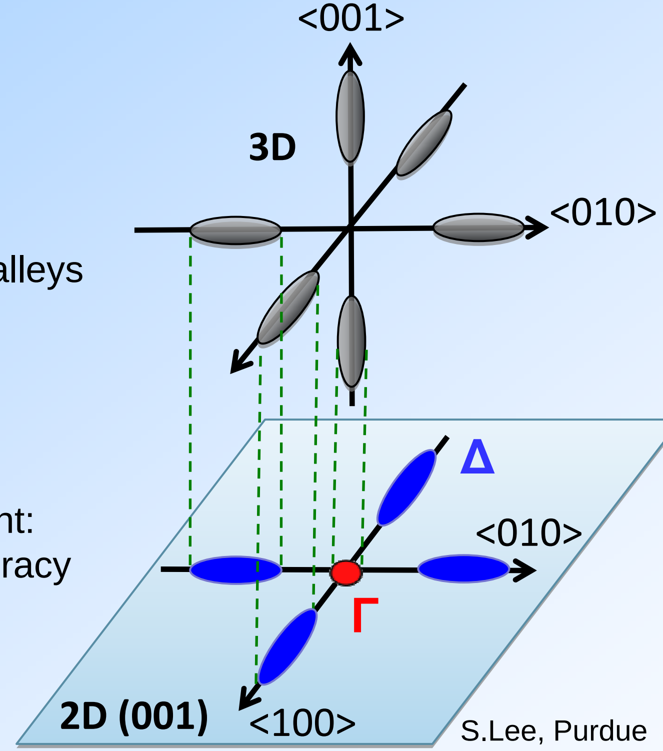
→ The tight lateral confinement of the leads cannot account for the dense excitation spectrum

Valley splitting in silicon devices

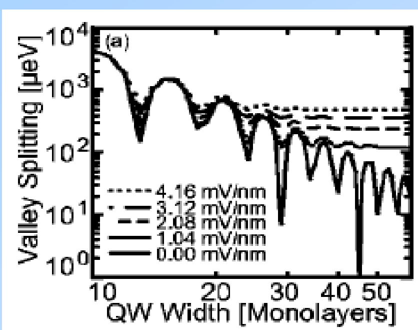


bulk Si:
6 degenerate valleys

strain, confinement:
2 + 4-fold degeneracy

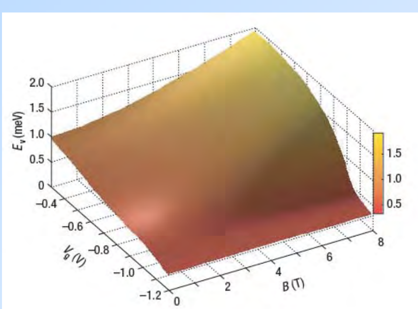


S.Lee, Purdue



Valley splitting oscillates as a function of well width

T. B. Boykin, *et al., Appl. Phys. Lett.* **84**, 115 (2004)

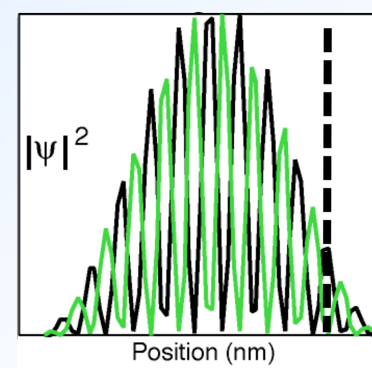


Valley splitting is controllable via gate voltage and B

S. Goswami, *et al., Nat. Phys*. **3**, 41 (2007)

steep confinement, interfaces:

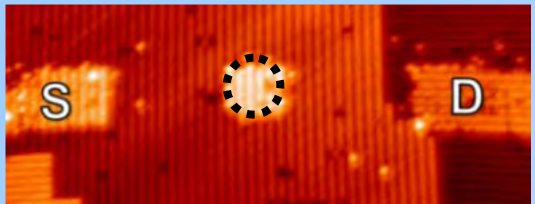
splitting of remaining degeneracy due to difference in fast oscillating part of the wave-functions

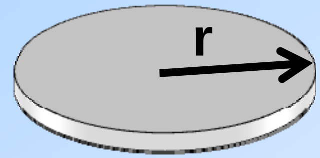


- valley splitting comparable in size to Zeeman splitting → valley states vs. spin states
- valley degeneracy can be a source of decoherence

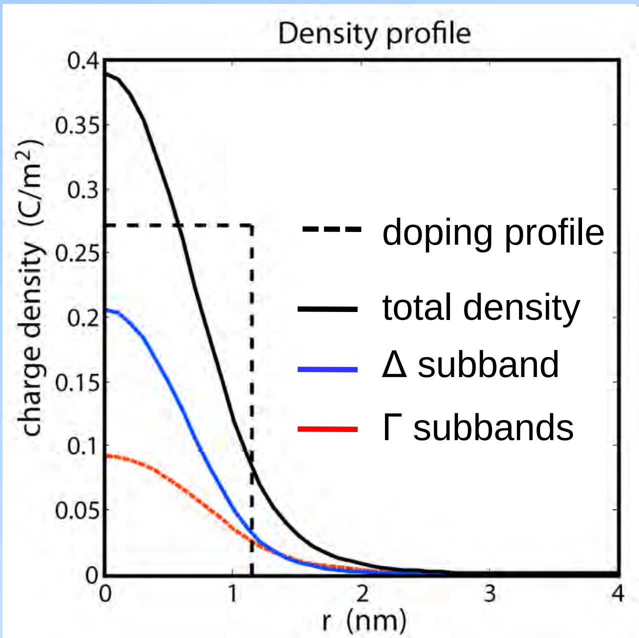
M. Friesen, *et al., Phys. Rev. B* **75**, 115318 (2007)
B. Koiller, *et al., Phys. Rev. Lett.* **88**, 027903 (2002)

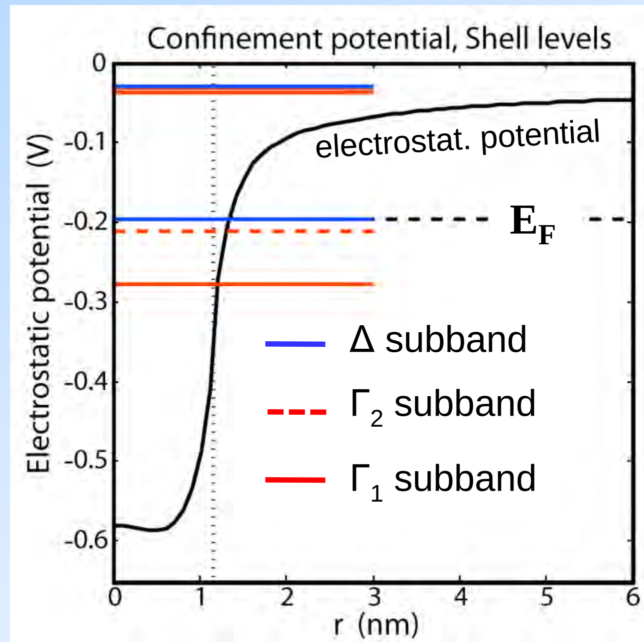
Effective mass modelling of 7 donor dot





σ = const, r =1.15nm



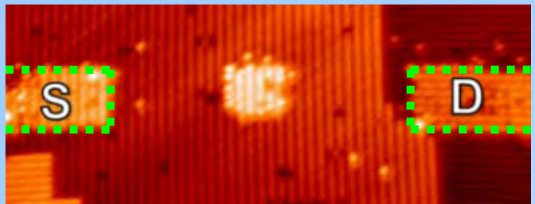


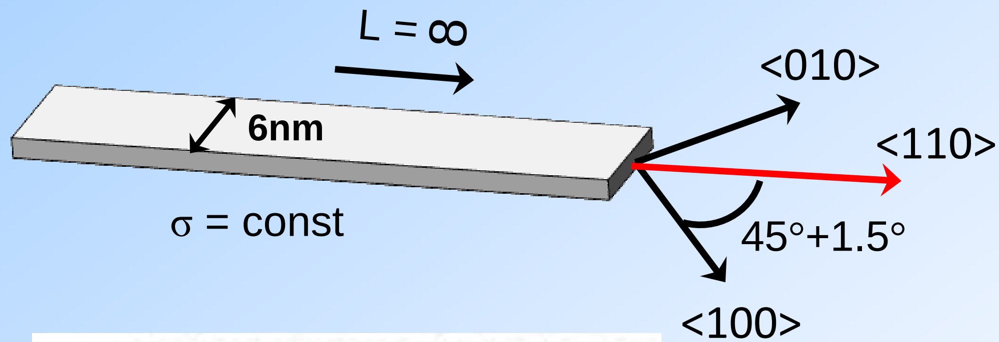
- Treat ions as 2D jellium of positive charge with circular symmetry
- Assume constant charge density from P δ-doped Si
- Self-consistently solve for charge density and energy levels using an effective mass approach

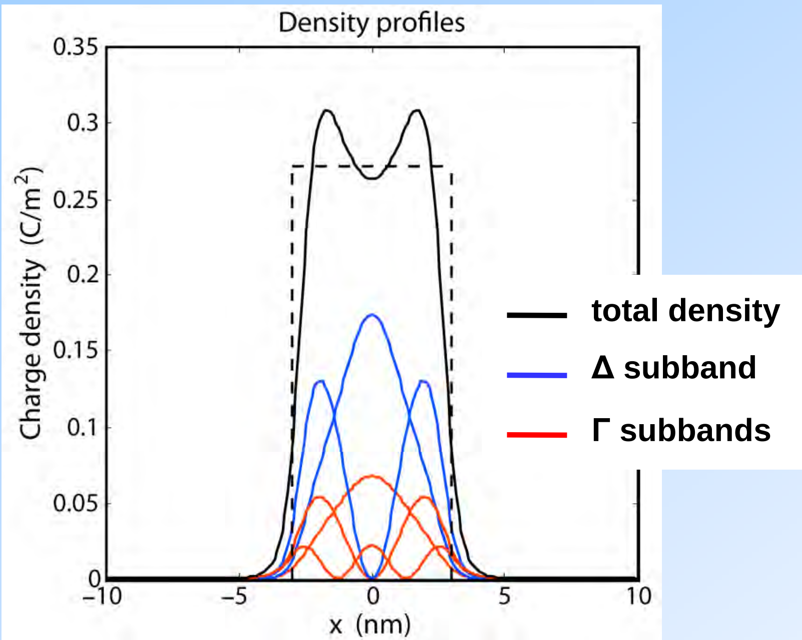
[$m^*_t = 0.21 m_e$ and $m^*_l = 0.95 m_e$
from G. Qian, *et al.*, *Phys. Rev. B* **71**, 045309 (2005)]

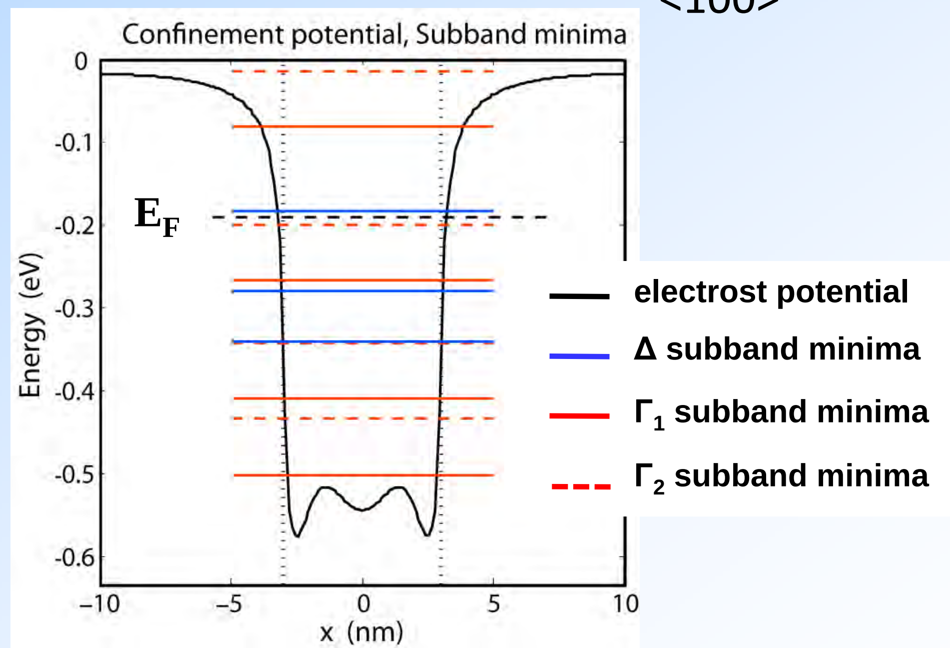
M. Friesen, M. Eriksson, Madison

Modelling of 1D source and drain leads









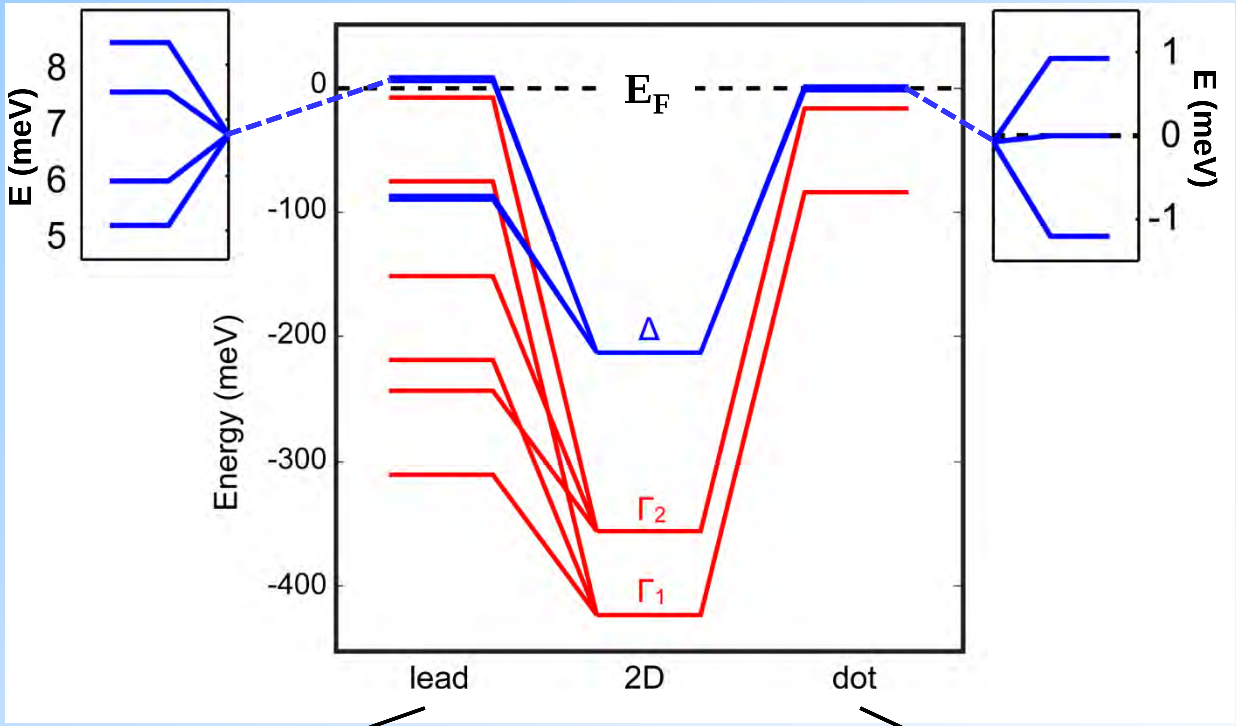
- Treat source and drain leads as an infinite 6nm wide wire
- Assumed orientation of 45 + 1.5 degrees from crystallographic [100] axes

M. Friesen, M. Eriksson, Madison

Comparison of 2D, 1D and 0D density of states in Si:P

(energy spectra aligned at their Fermi levels)

Valley degeneracies lifted due to 1.5° misalignment from [110]



middle level 2-fold degenerate due to circular symmetry

- Subband spacing on the order of 10s of meV
- It is unlikely that the valley split Δ states are aligned exactly at E_F to contribute to observed low-lying spectrum

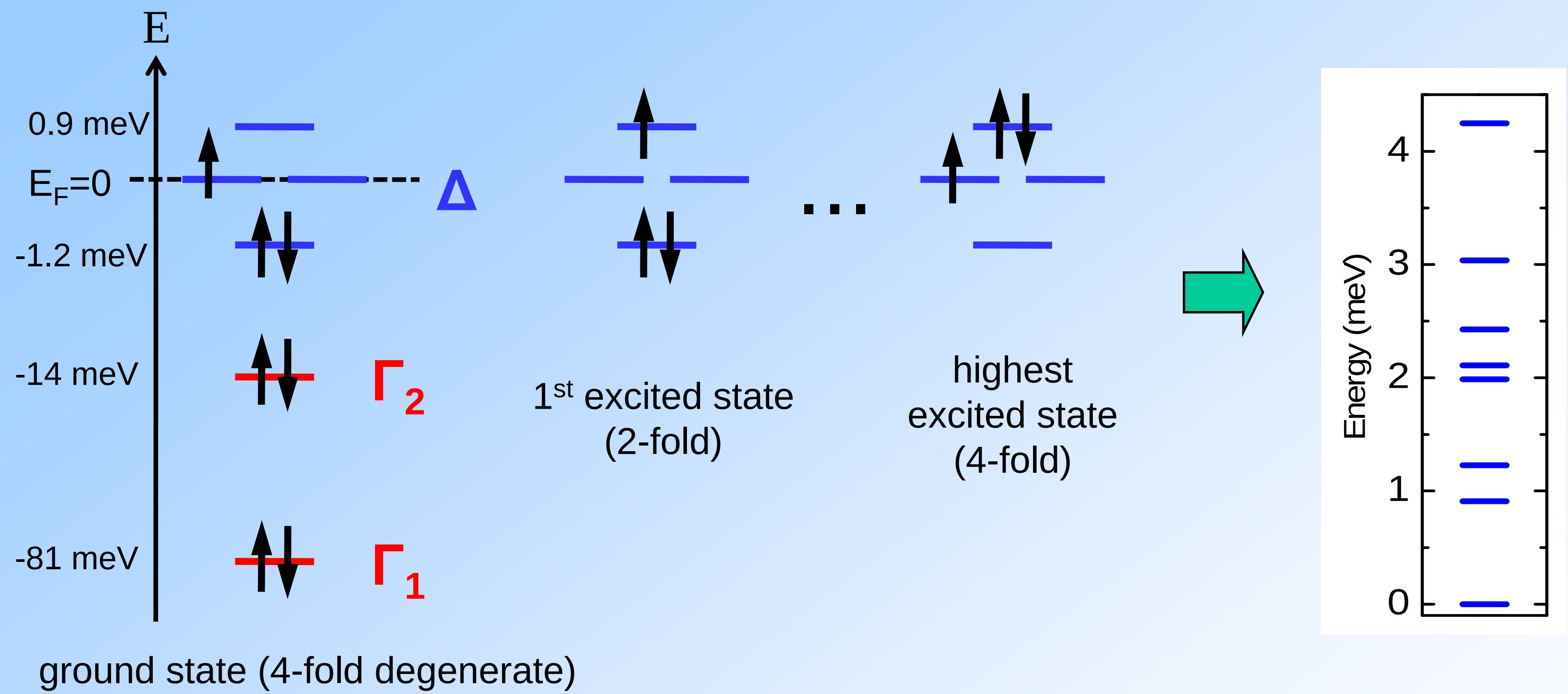
- 3 "shells" occupied: Γ_1, Γ_2 and Δ
- Valley splitting of Δ states on the order of 1meV at E_F

➔ The observed spectrum at small bias voltages is due to electronic states in the leads

D. Carter, *et al. Phys. Rev. B* **79**, 033204 (2009)

M. Friesen, M. Eriksson, Madison

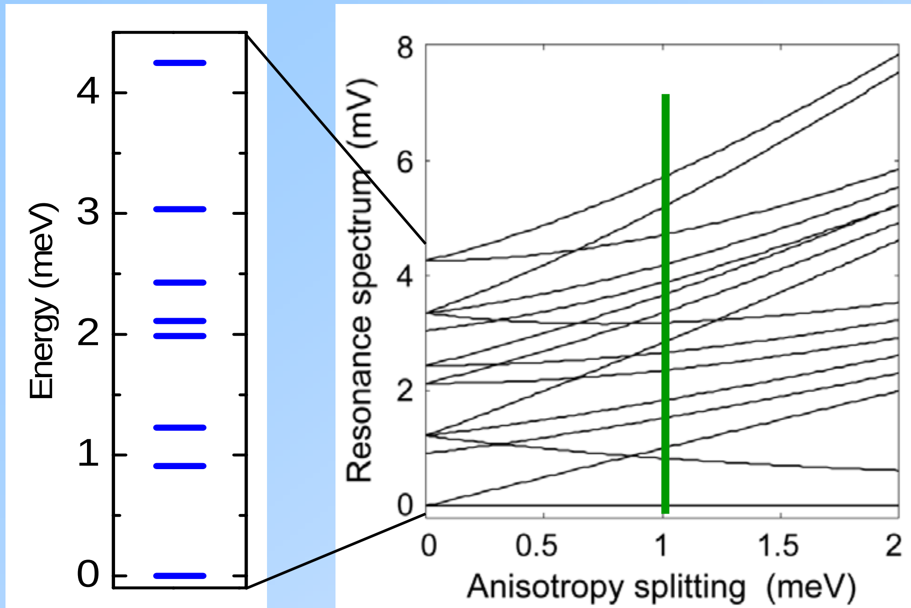
Calculated transport spectrum of a 7 donor symmetric dot

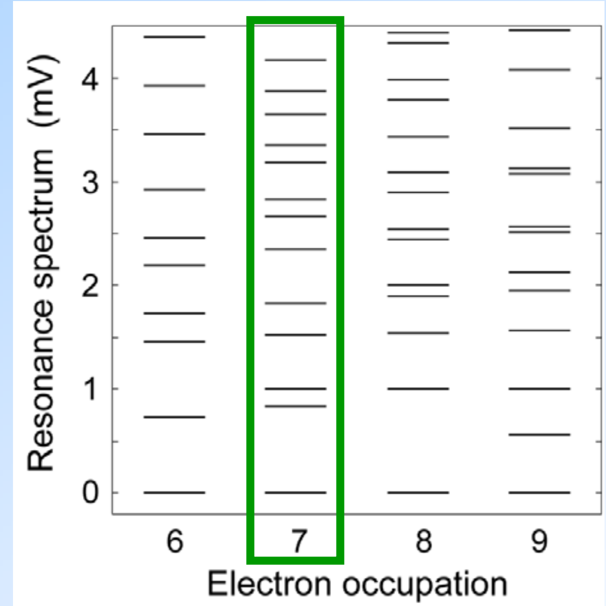


- For 3 electrons in Δ shell: there are 56 possible configurations with 8 different energies (2 to16-fold degenerate)
- In addition, all levels are 2-fold spin degenerate

➔ For N=7: around zero bias there are 8 transport resonances within ~4mV bias window

Realistic asymmetric dot: splitting of remaining degeneracy





Modelling: avg. level spacing ~300μeV

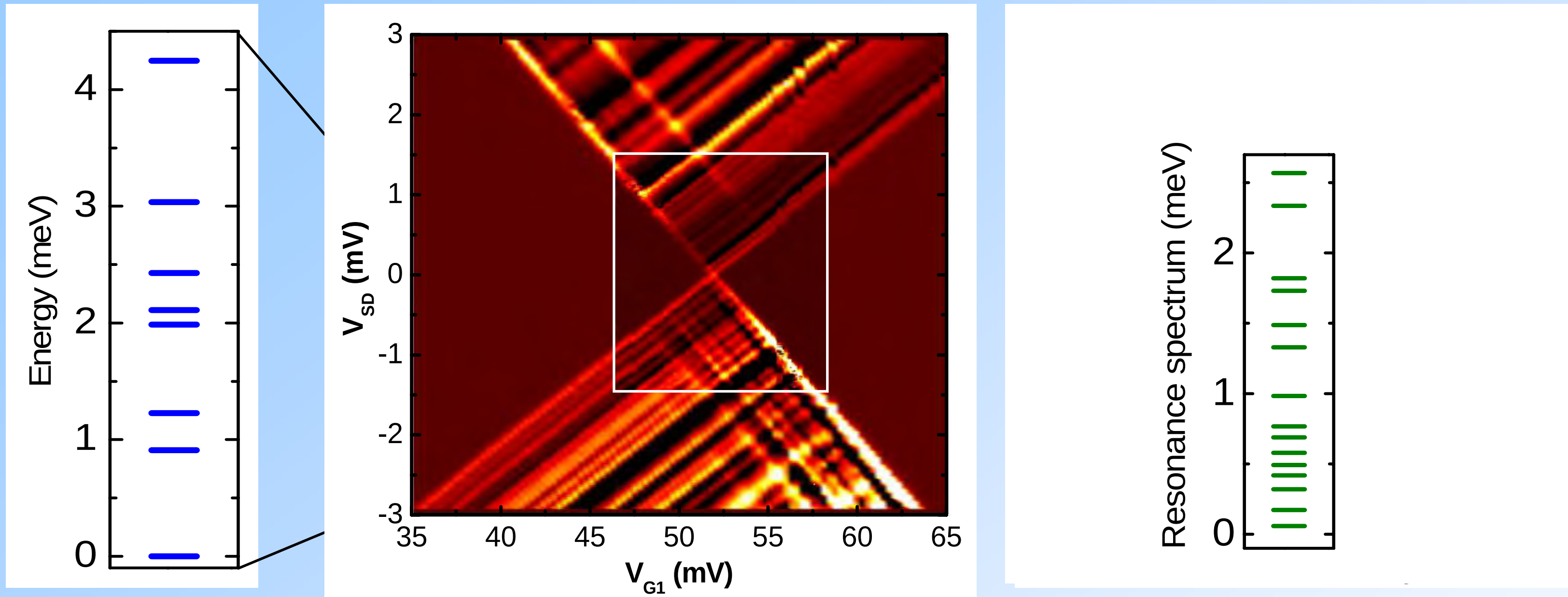
- We use a perturbation approach to include dot anisotropy

➔ The remaining degeneracies are lifted (except for spin)

➔ Good qualitative agreement with the observed spectrum

➔ **The observed resonances are due to valley splitting in the quantum dot**

Realistic asymmetric dot: splitting of remaining degeneracy



Modelling: avg. level spacing ~300μeV

Experiment: avg. level spacing ~100μeV

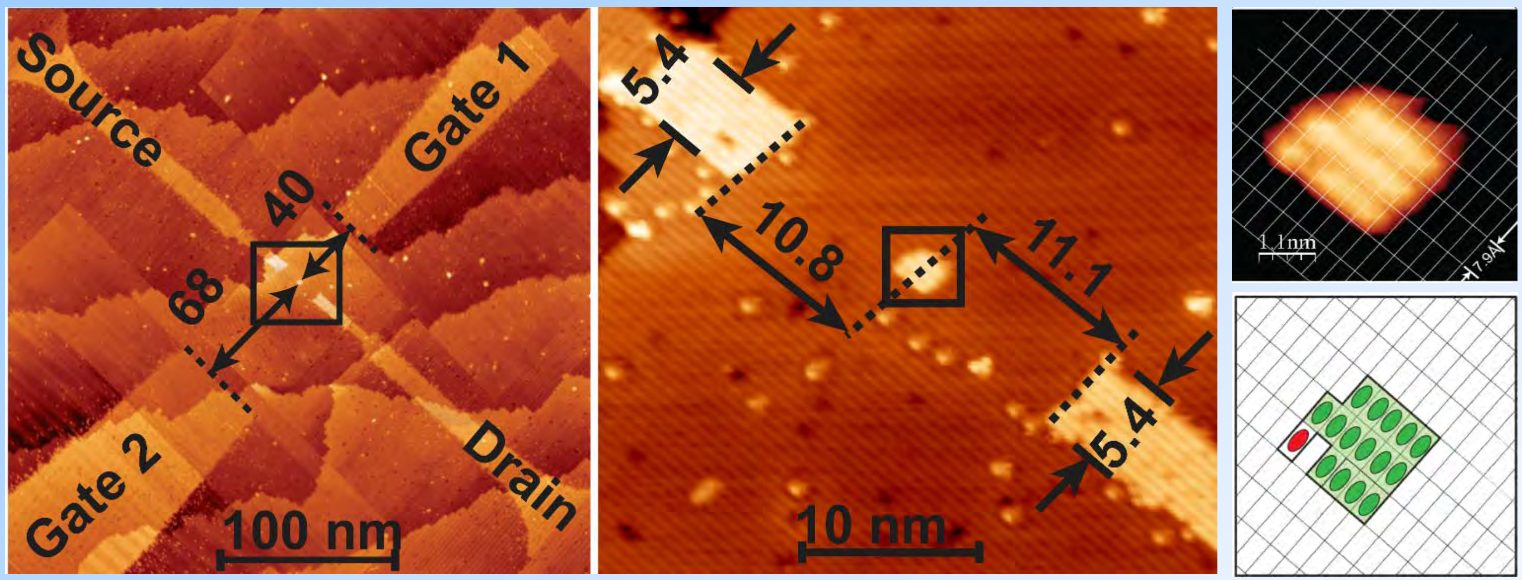
- We use a perturbation approach to include dot anisotropy

➔ The remaining degeneracies are lifted (except for spin)

➔ Good qualitative agreement with the observed spectrum

➔ **The observed resonances are due to valley splitting in the quantum dot**

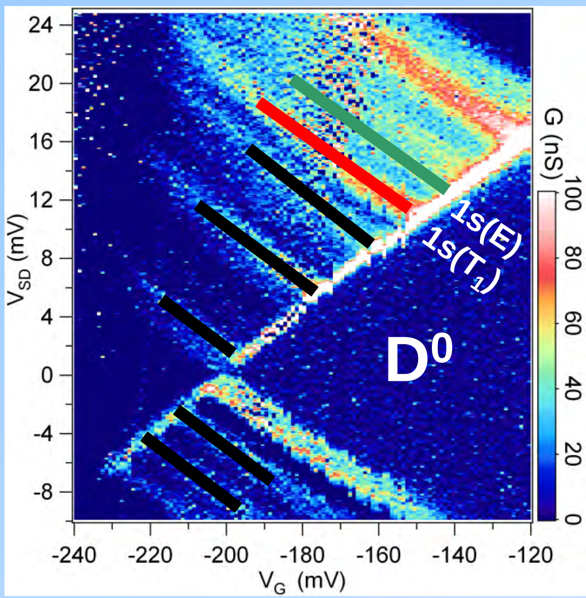
How does the valley splitting change in the single donor limit?

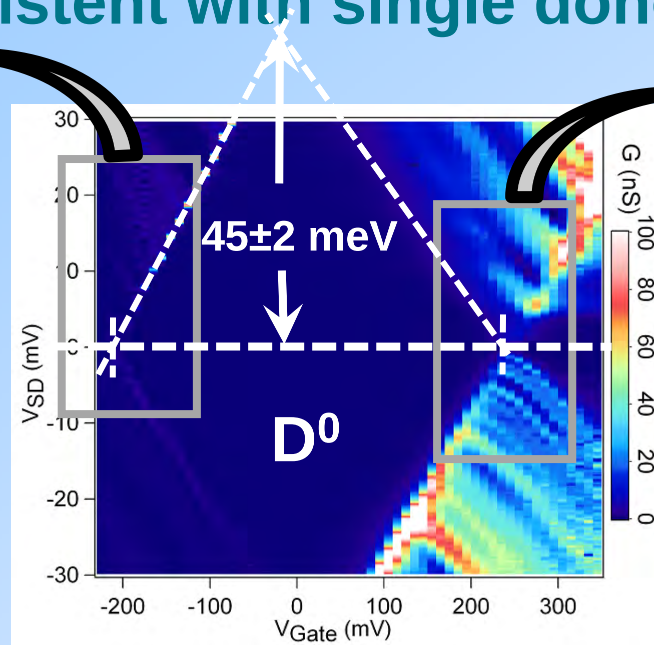


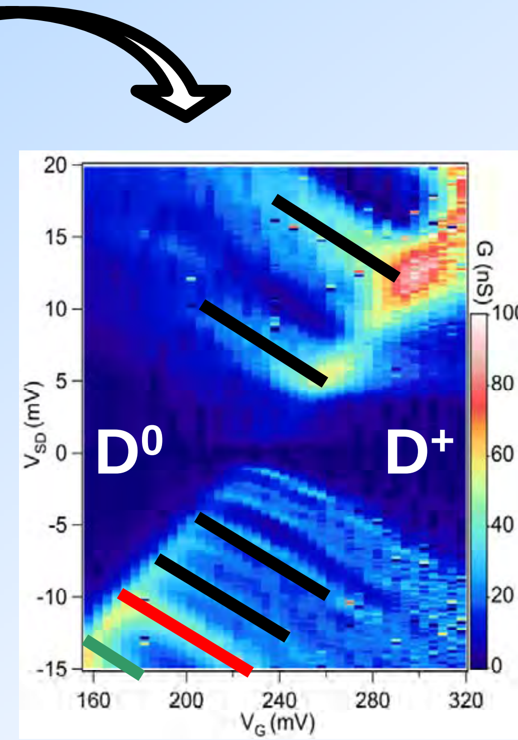
- We have a decreased the desorbed dot area (1.7 x 1.7 nm^2)
- From desorption statistics:

➔ 1-3 donors most probable due to edge effects

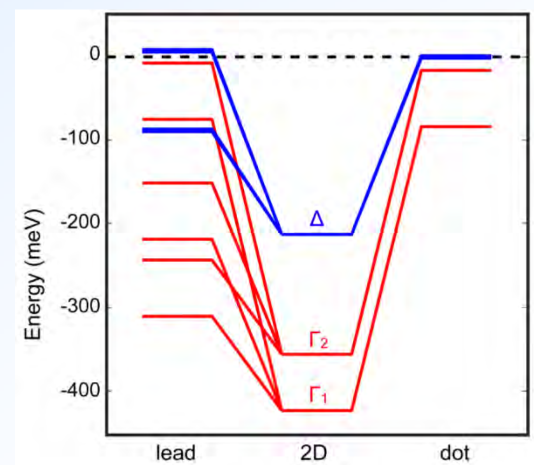
Spectroscopy consistent with single donor





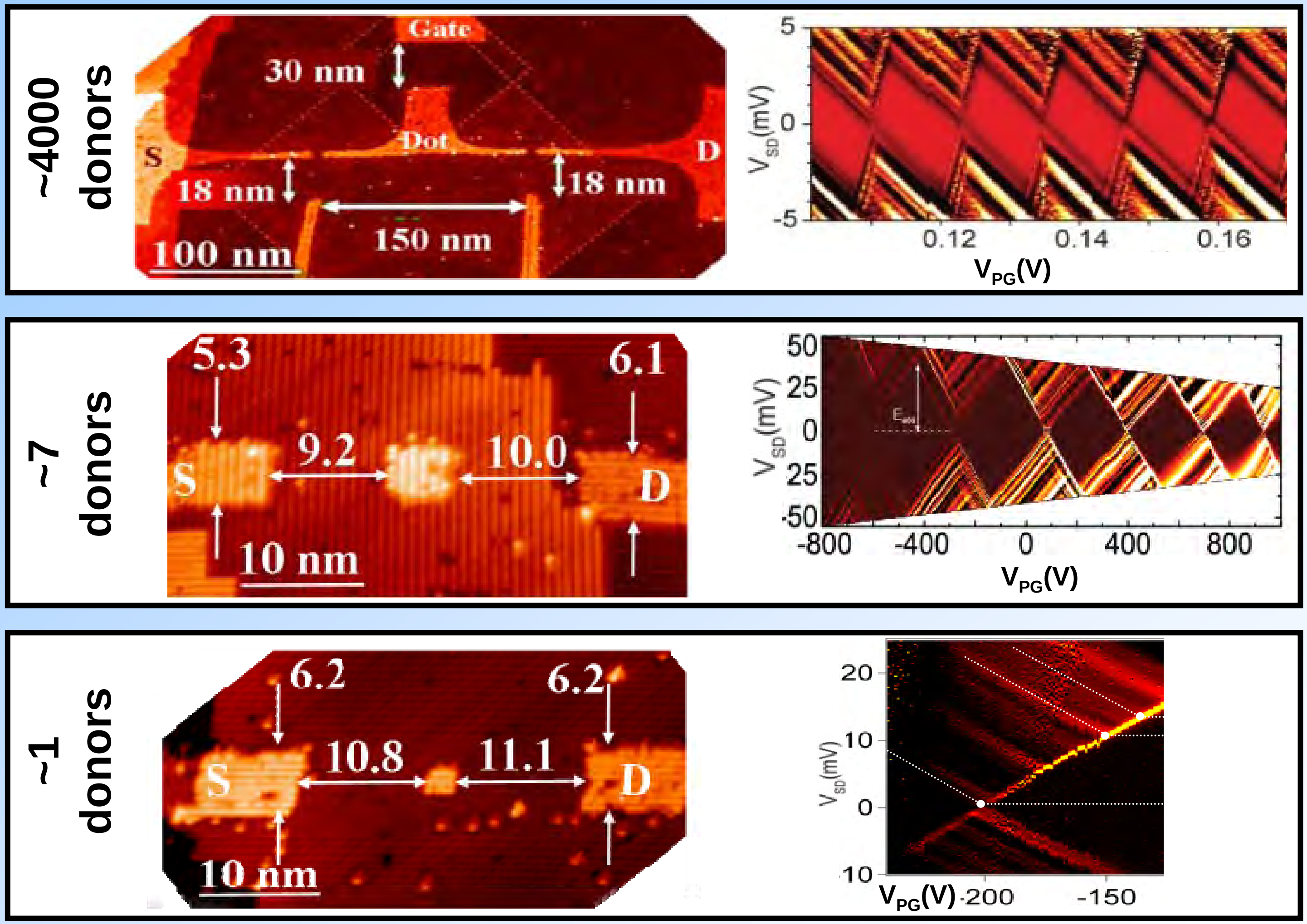


Excited States	1s(T1)	1s(E)
Bulk Si:P (mV)	11.70	13.01
(+)ve VG1 (mV)	10.4±2.8	13.8±1.4
(-)ve VG1 (mV)	10.8±1.3	13.9±1.4



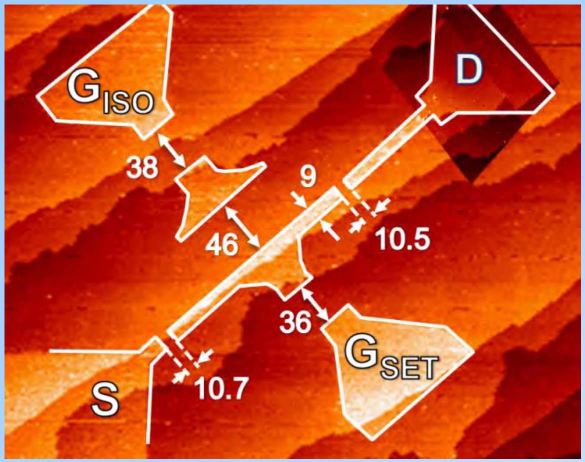
- The addition energy is consistent with the D^0 ground state of a P donor
- The excited state resonances are consistent with transitions of a single P donor in bulk Si (visible at either end of the D^0 diamond)
- Additional lines may be due to van Hove singularities of the leads

Valley splitting in donor based quantum dots

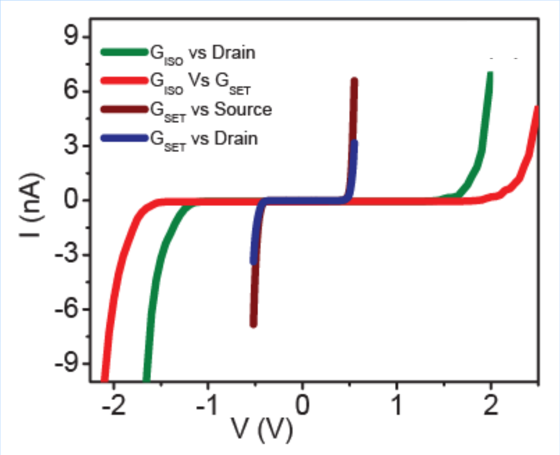


➔ **modeling provides consistent explanation for all transport resonances observed**

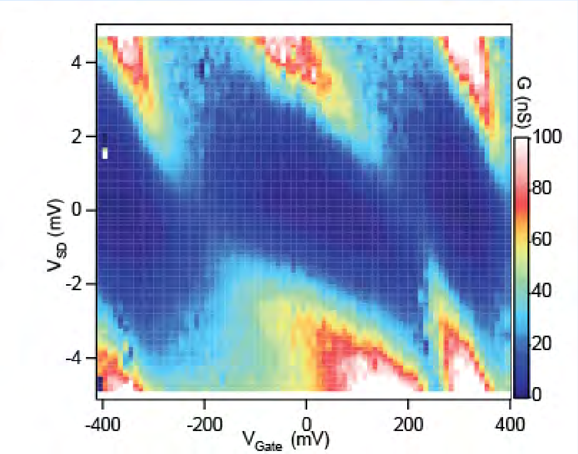
Towards charge detection in an in-plane architecture



parallel double dot structure



gate leakages



stability diagram of SET dot at 4K

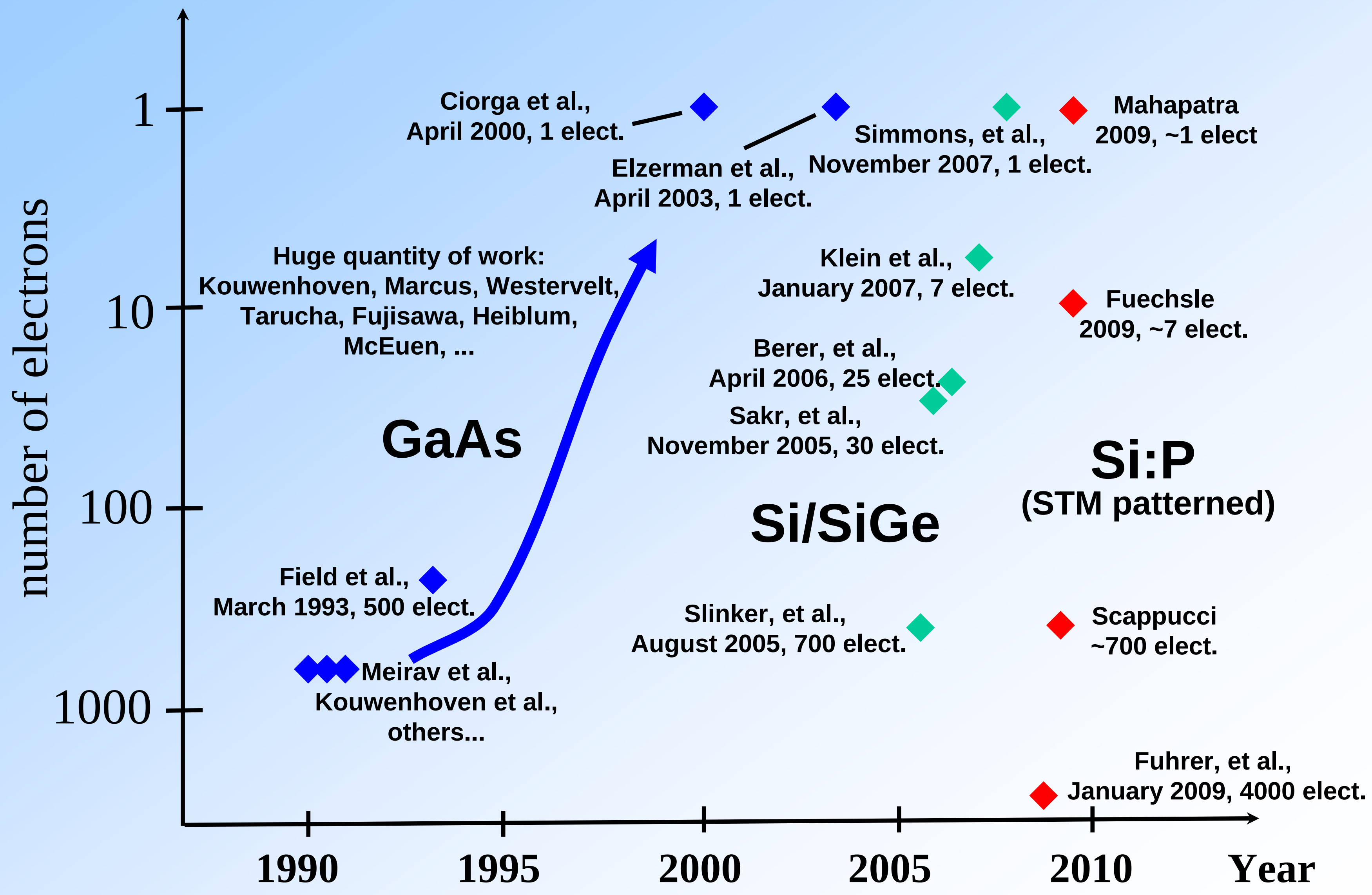
- We demonstrate the ability to pattern a second quantum dot as a SET detector
- The gating ranges match with device design
- The SET charging energy is in agreement with FastCap calculations (≤ 5meV)

➔ Further optimization of the device design is necessary

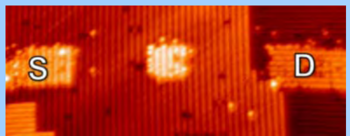
F. Hofmann, *et al., Phys. Rev. B* **51** (1995)

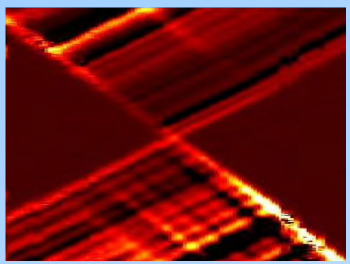
Number of electrons in gated quantum dots

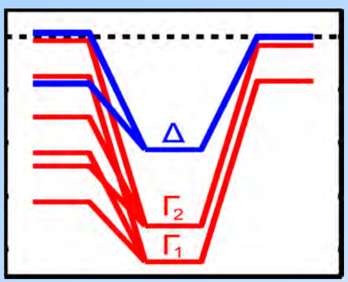
(courtesy of M. Eriksson)

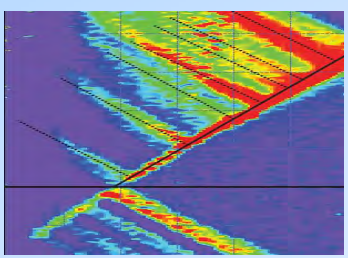


Summary









- We have decreased the number of donors from 4000 to ~1
- Valley splitting leads to a dense excitation spectrum in a 7 donor based quantum dot with an energy of 100μeV
- This splitting is reduced at the level of single donors.
- Effective mass theory provides an efficient means to analyze complex donor structures in silicon
- Strategies underway to control valley splitting: using lower carrier densities and strain.
- We have demonstrated the integration of a second dot towards the goal of an in-plane charge sensor