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High precision quantum device modeling using the atomistic tight-binding technique

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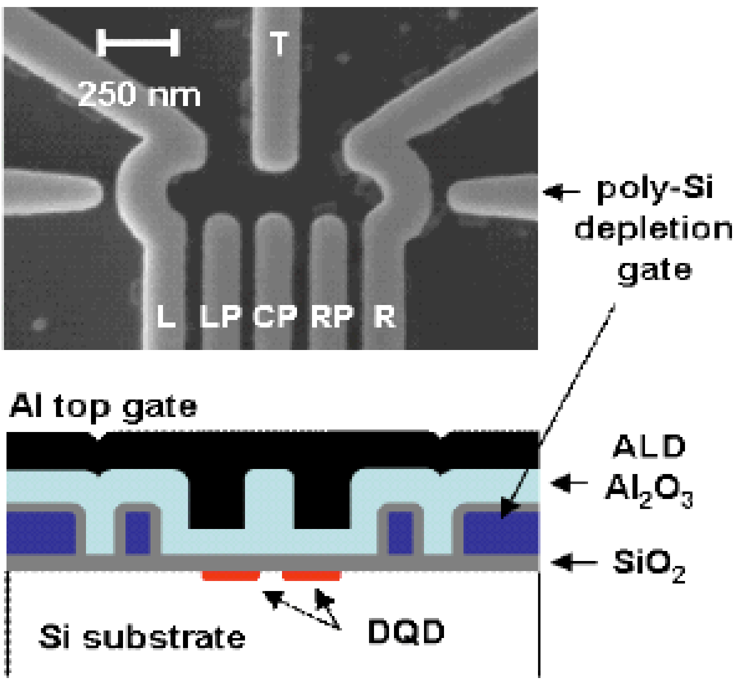
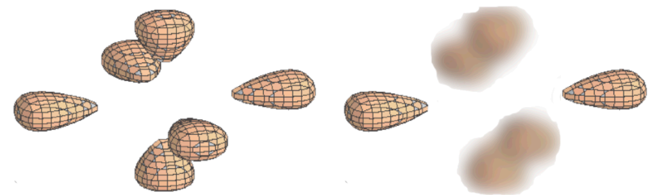
Si Quantum electronics

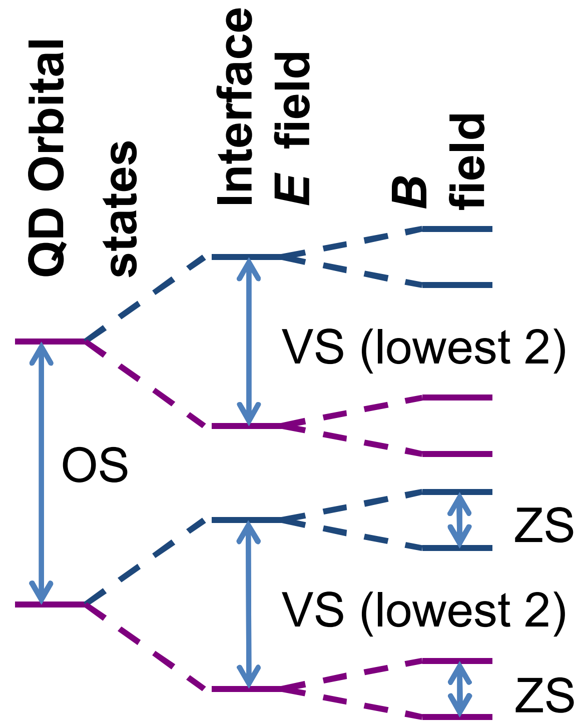
SNL QIST: DQD S-T Qubits in Si



Tracy et. al., APL 97, 192110 (2010)

CB valleys in Si: 2-4 splitting





Method: TB+FCI

Good 1e wfs + Full CI for few electrons

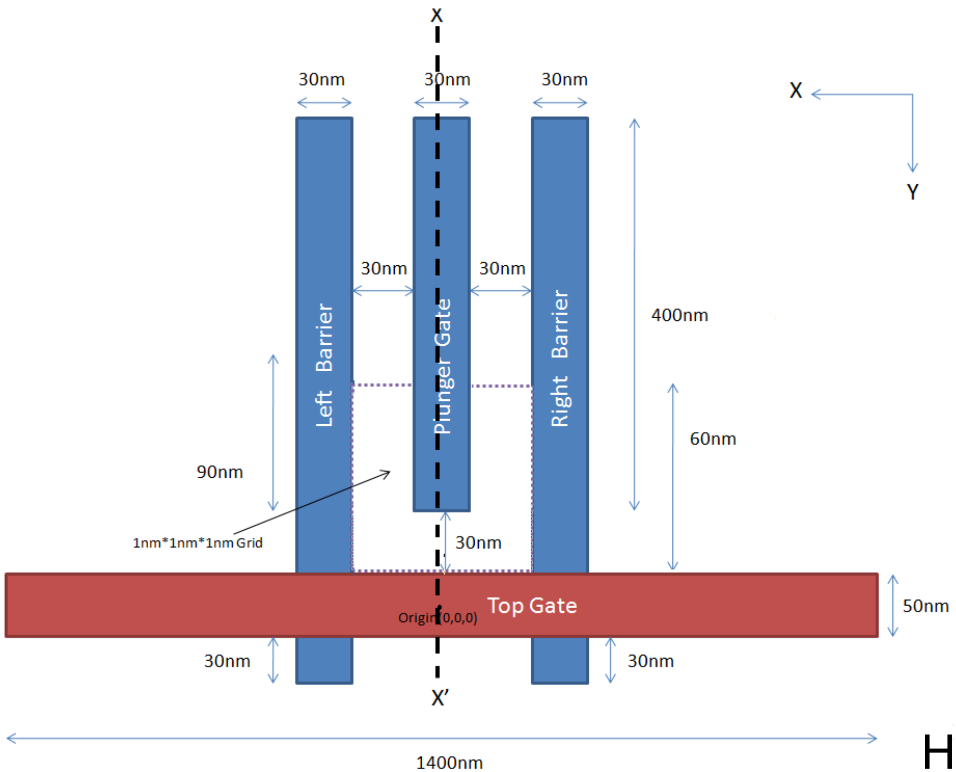
Atomistic tight-binding (NEMO 3D)

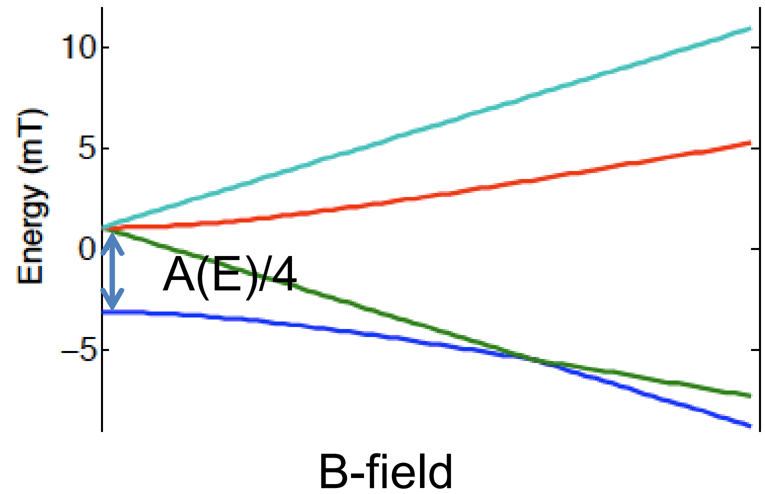
- LCAO, full bandstructure method (no extra parameter for VS)
- miscut (tilt)
- surface roughness
- alloy disorder
- strain
- hetero-structures
- realistic device geometries
- E-fields
- B-fields
- multi-million atom systems (HPC)

Configuration Interaction
E. Nielsen, et. al. PRB 82, 075319 (2010).

- Few electron full Hamiltonian
- J, K in k-space
- Computational speed (HPC)

1. Hyperfine Stark Effect (CQC2T)





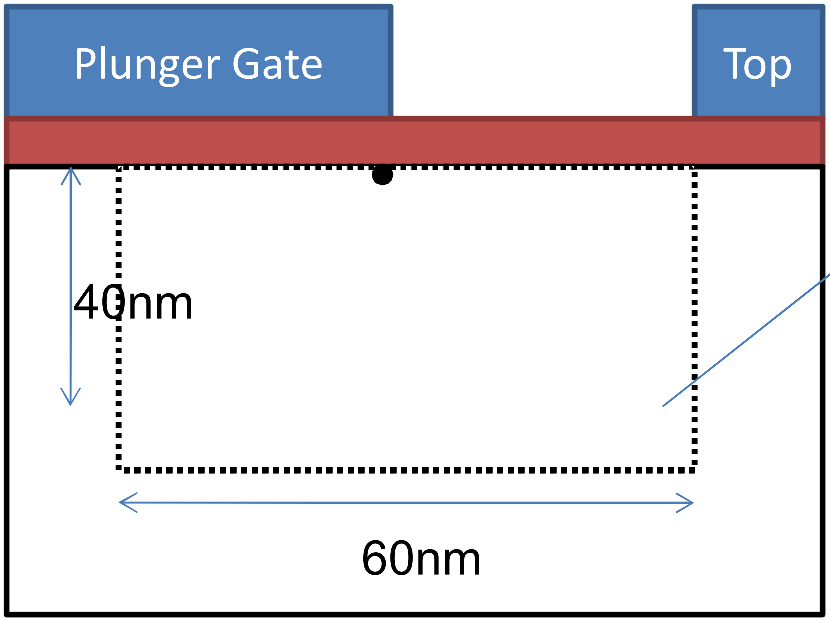
$A(E) \longrightarrow |\Psi(E, r_0)|^2$

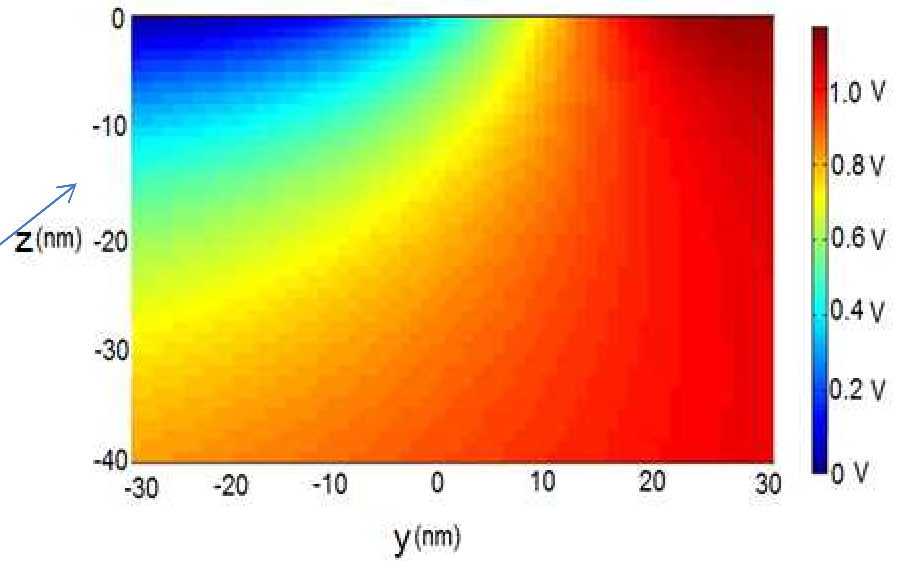
Hyperfine resonance measured: 2.8 mT

Hyperfine resonance of bulk P: 4.2 mT

Collaboration: F. Mahiyaddin, A. Morello, A. Dzurak, L. Hollenberg

Hyperfine Stark Effect (CQC2T)

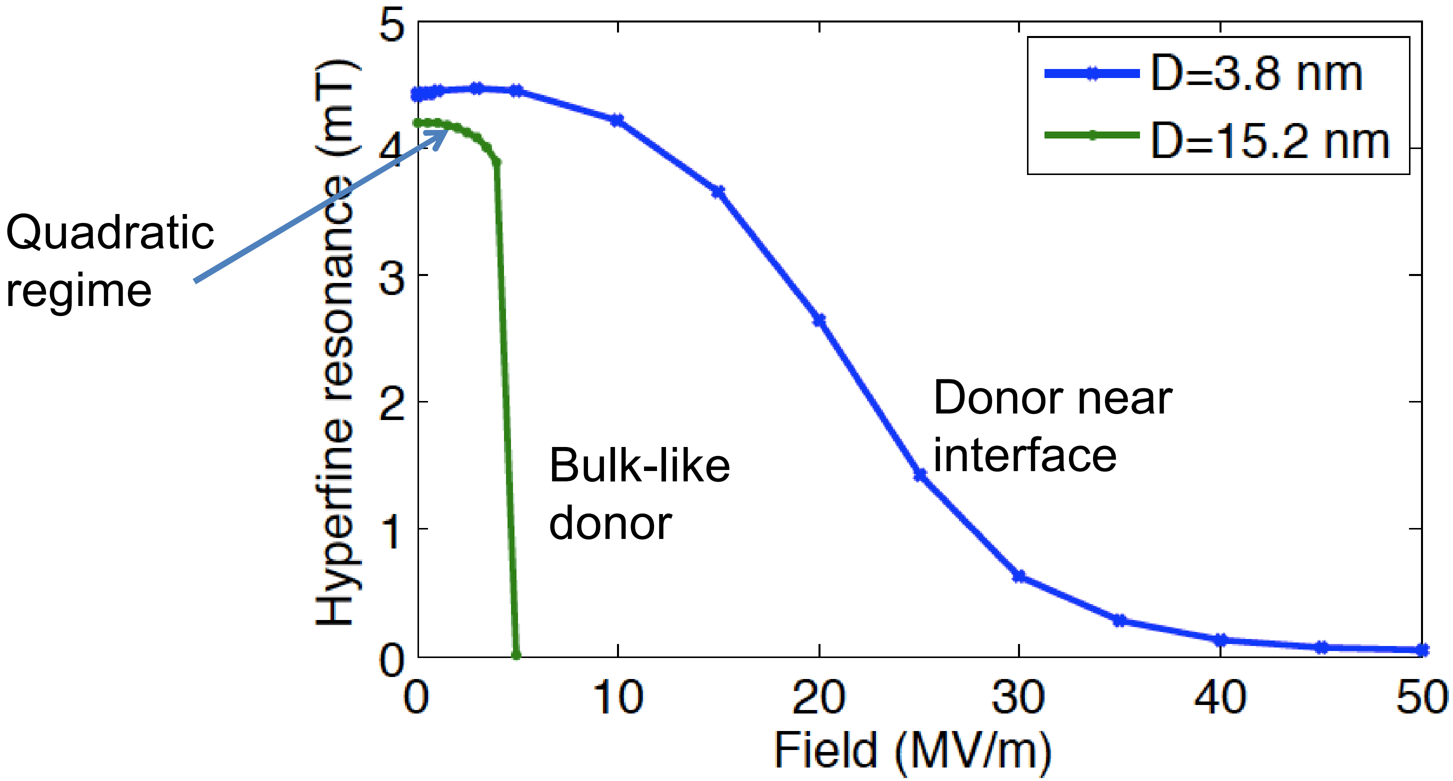




NEXT_NANO (3D potential)

Top Gate = 1.5V
Plunger Gate = -1.875V
Barriers – 0.625V

High Field Hyperfine Stark Effect

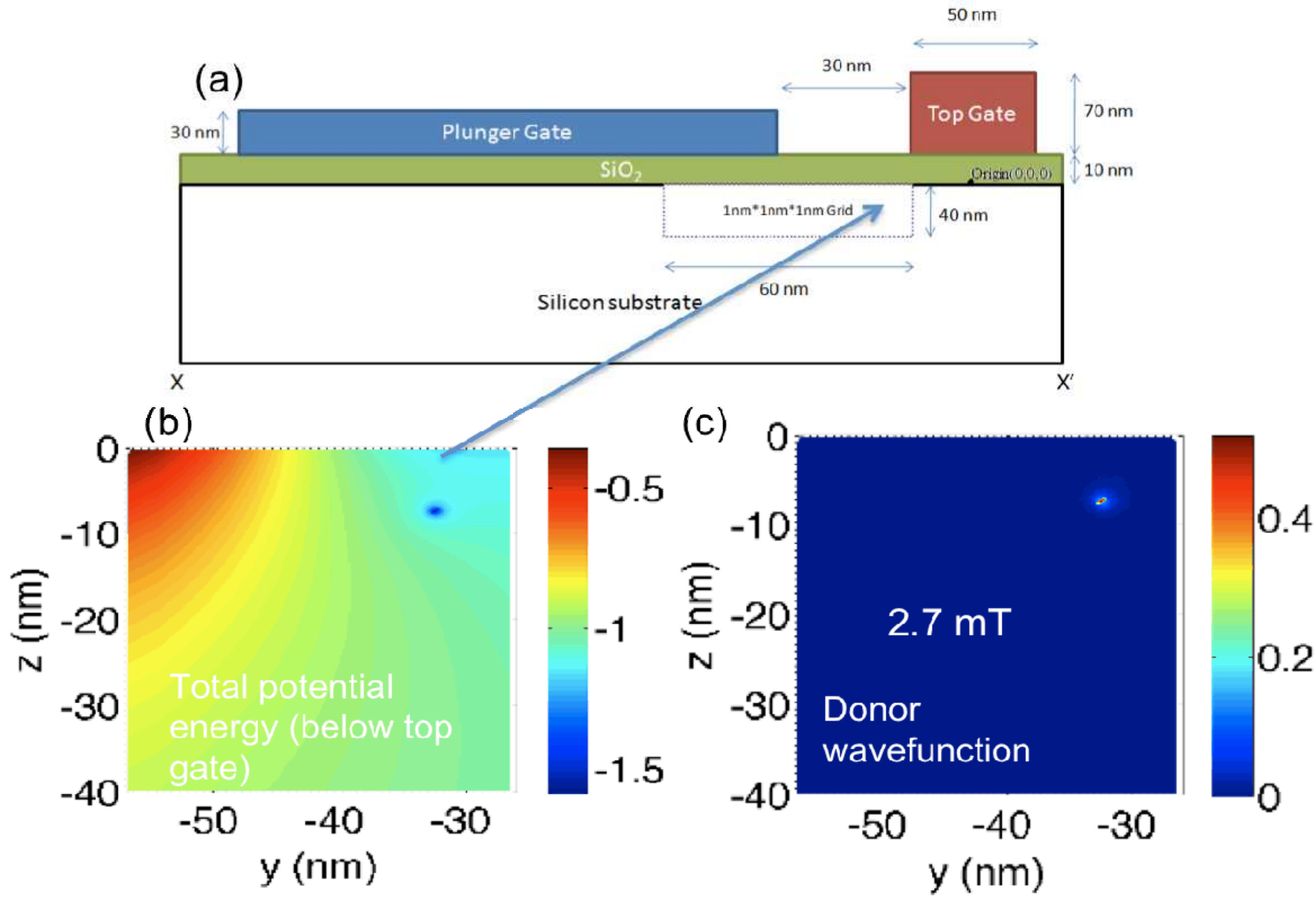


Theory: Rahman et al. PRL 99, 036403 (2007)

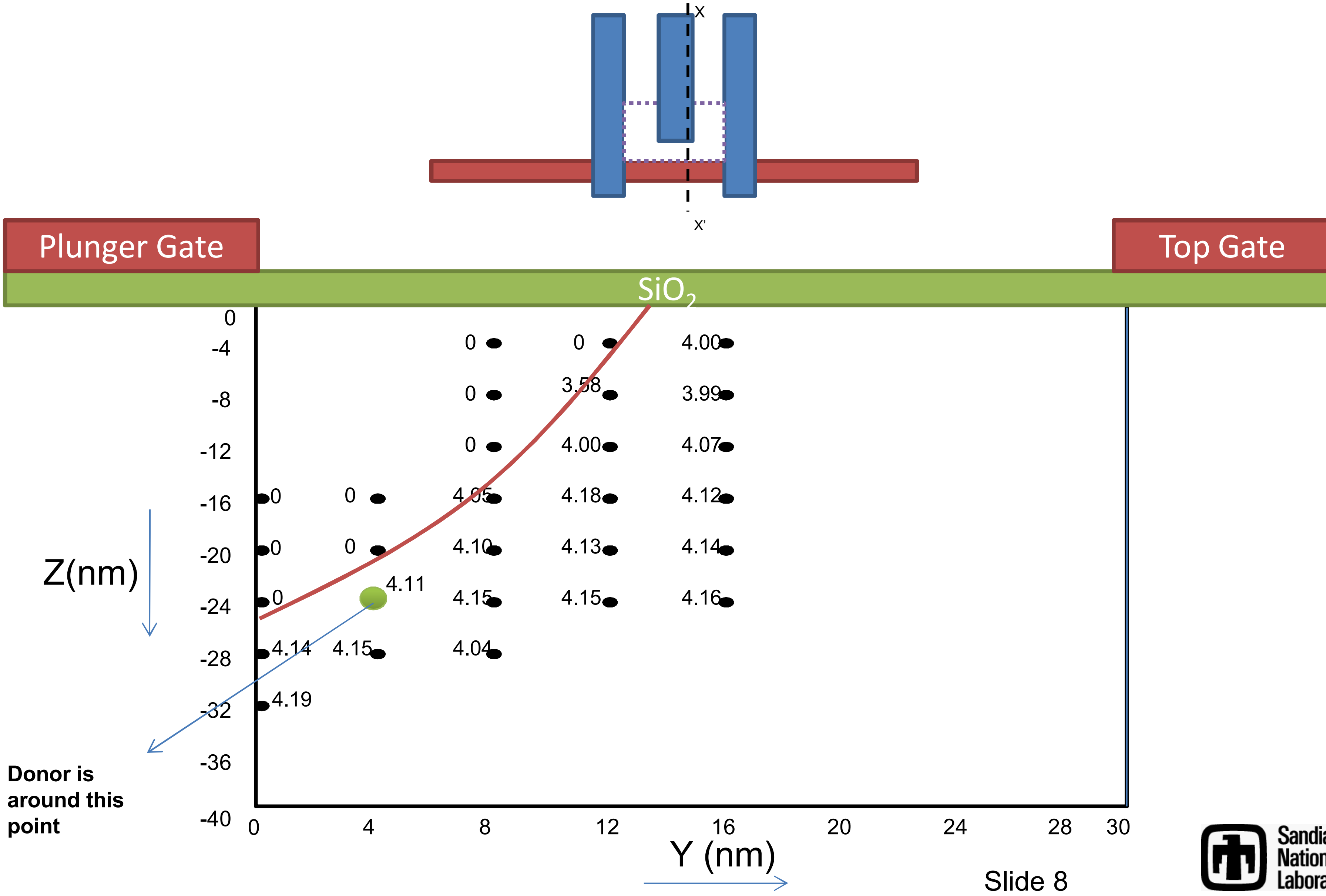
High-field regime accessible due to surface hybridization

Bulk donors – ionization limited

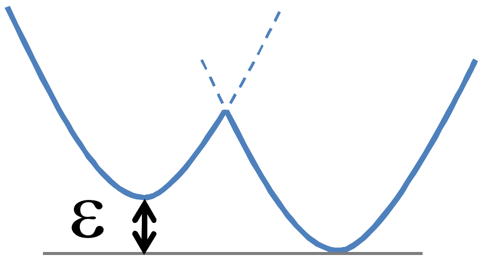
CQC2T measurements explained



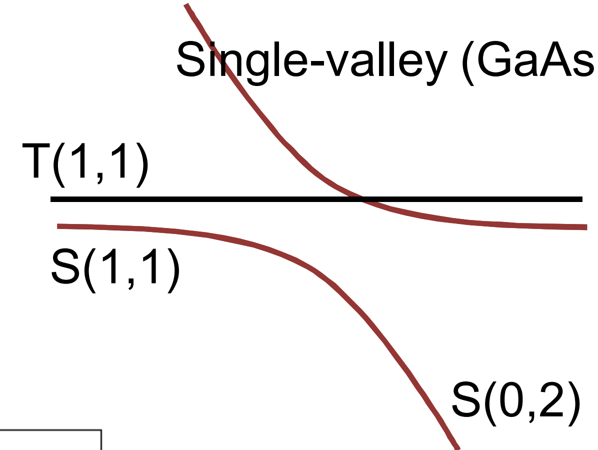
Device 1 – Contact Hyperfine (mT) at different locations of donor
Slice x at 10 nm from centre of plunger towards barriers

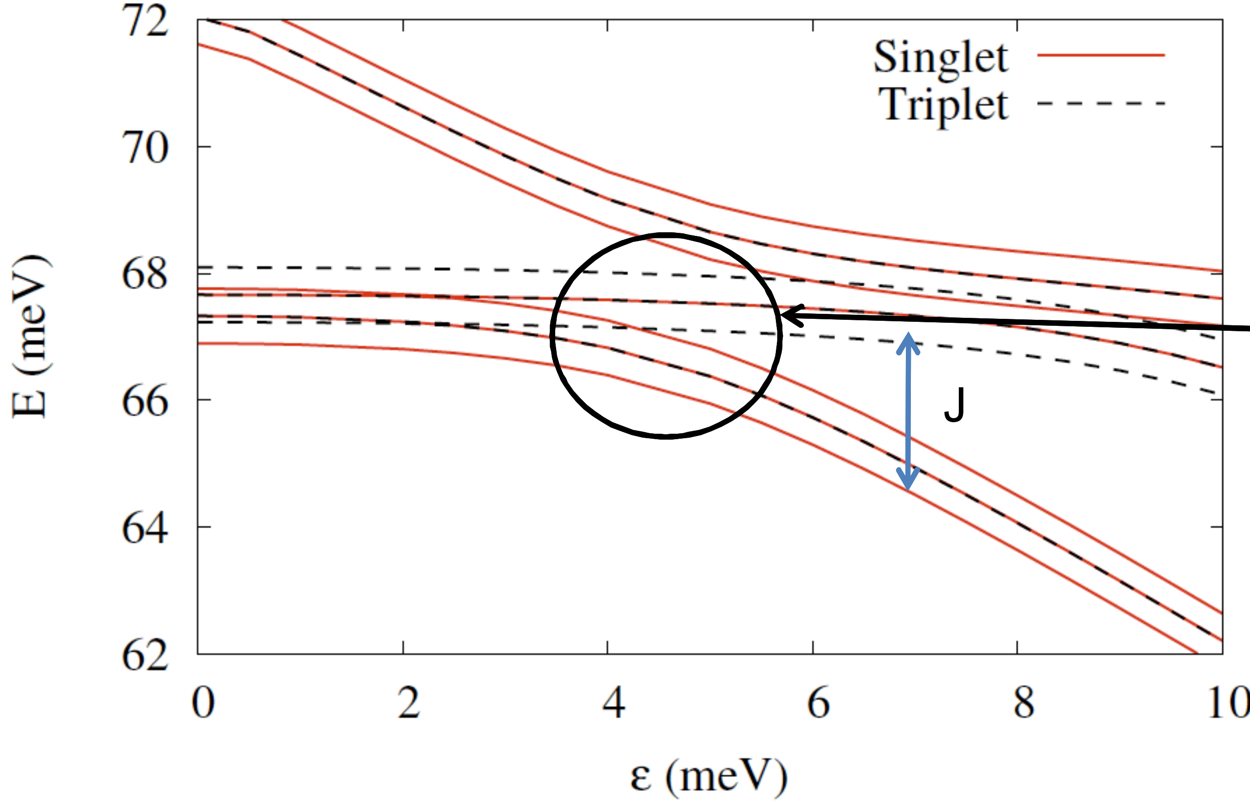


2. Ideal DQD 2e states (NEMO+CI)



TB+CI





Multiple singlets and triplets with small valley coupling (E. Nielsen)

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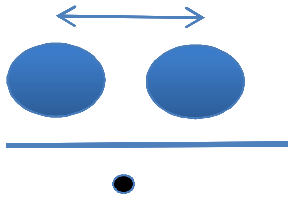
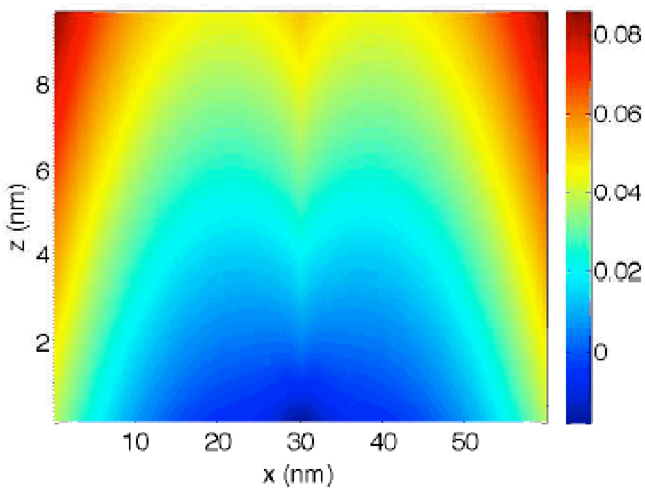
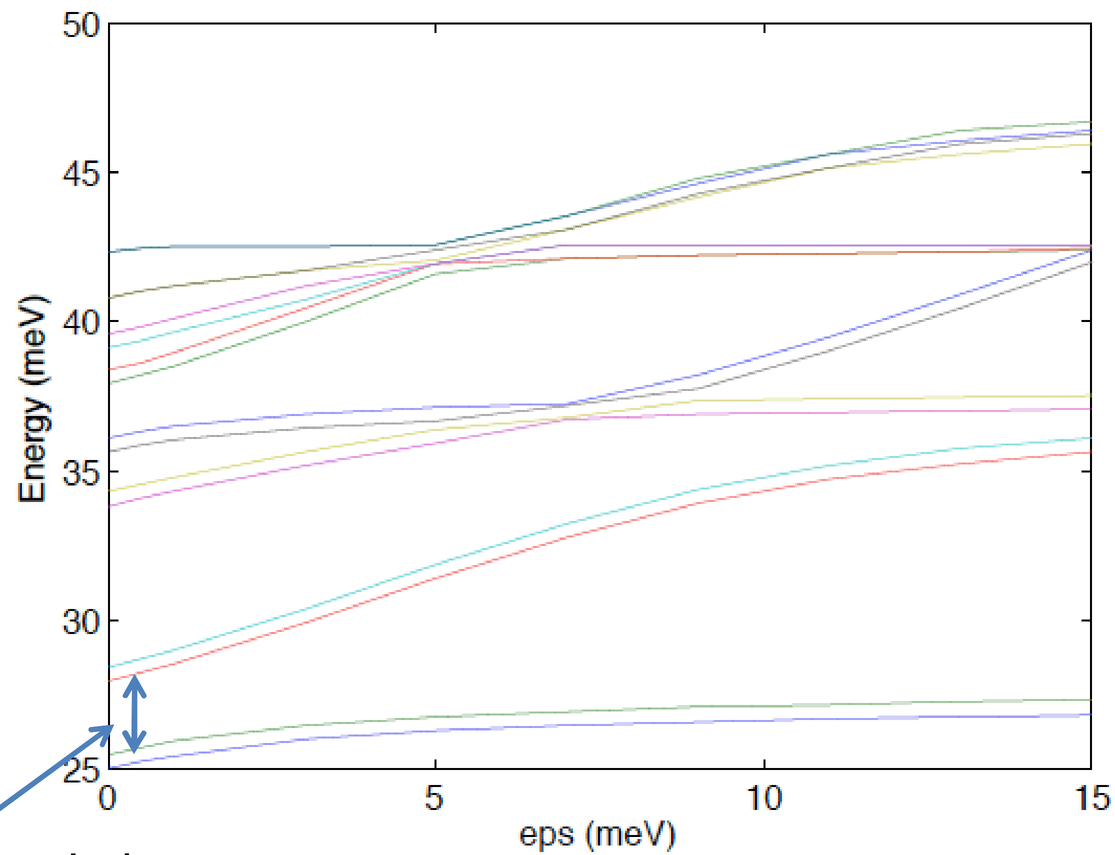
Defect at tunnel barrier (1e states)

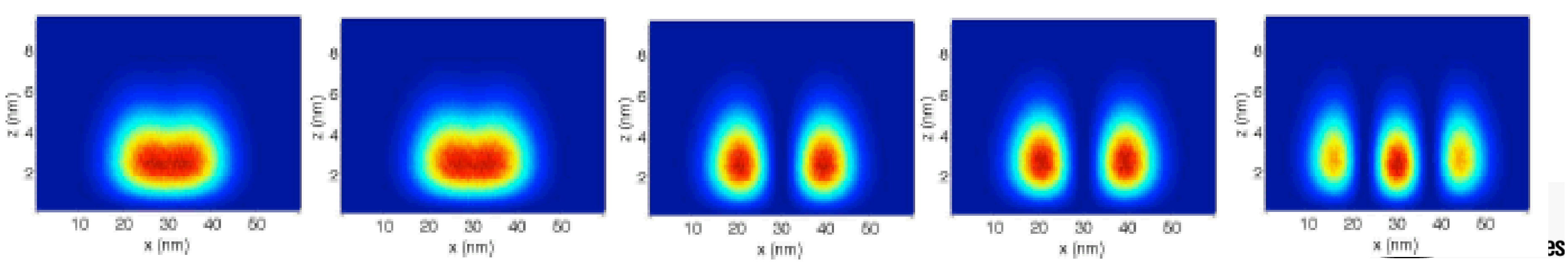


potential

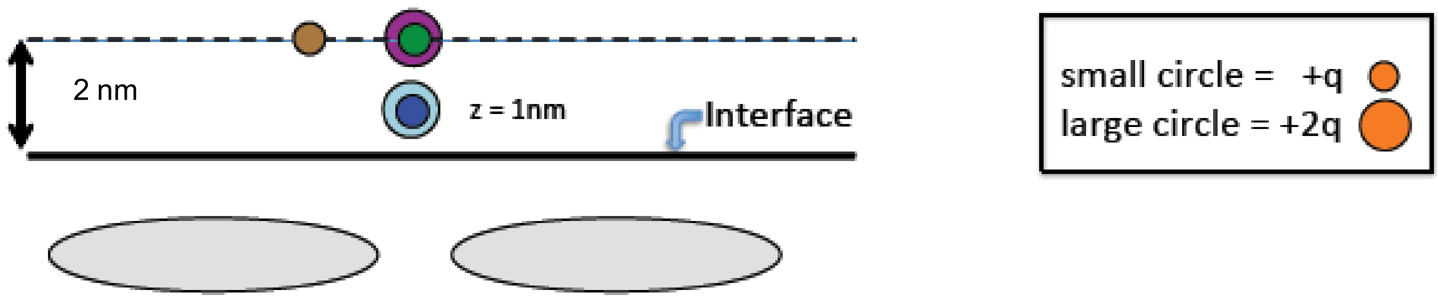




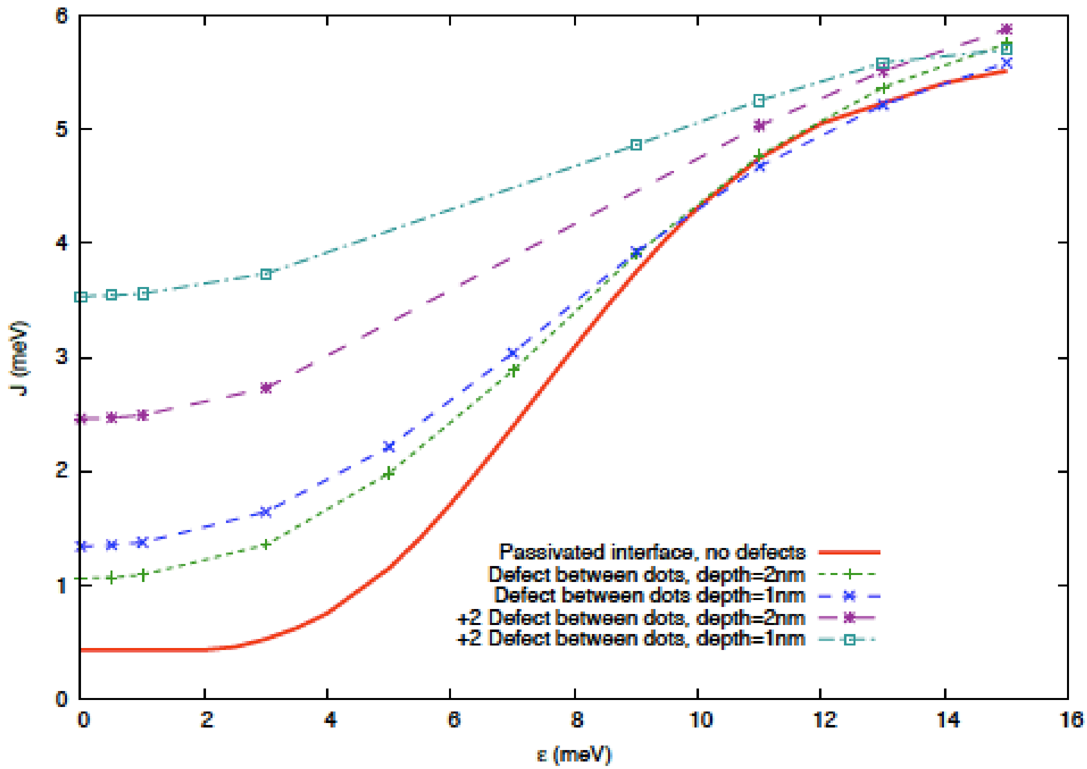
Tunnel coupled gap



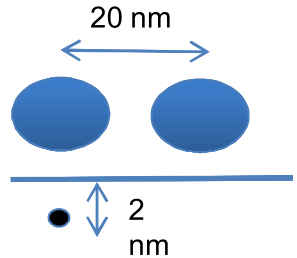
Defect at tunnel barrier between dots

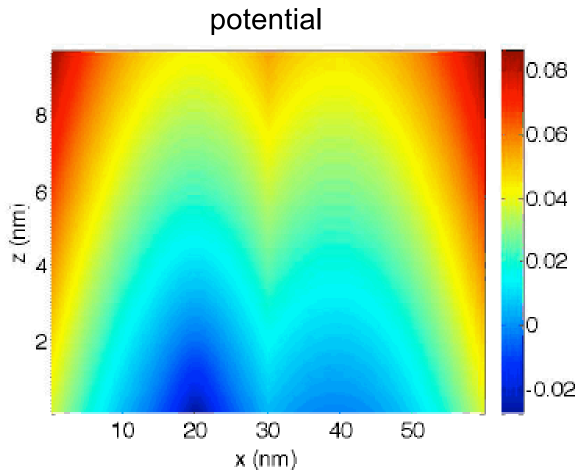


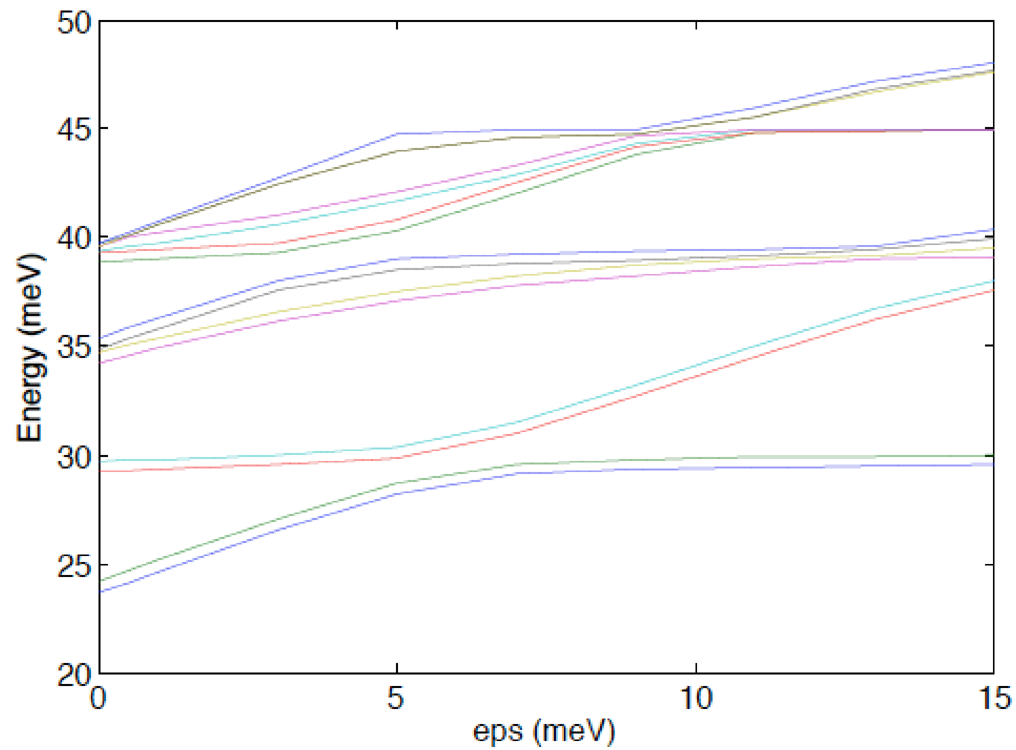
- Curve flattens as tunnel barrier is lowered
- Exchange at zero detuning increases
- J curve is sensitive to defect depth and magnitude
- Defects in the barrier can make it hard to form a DQD

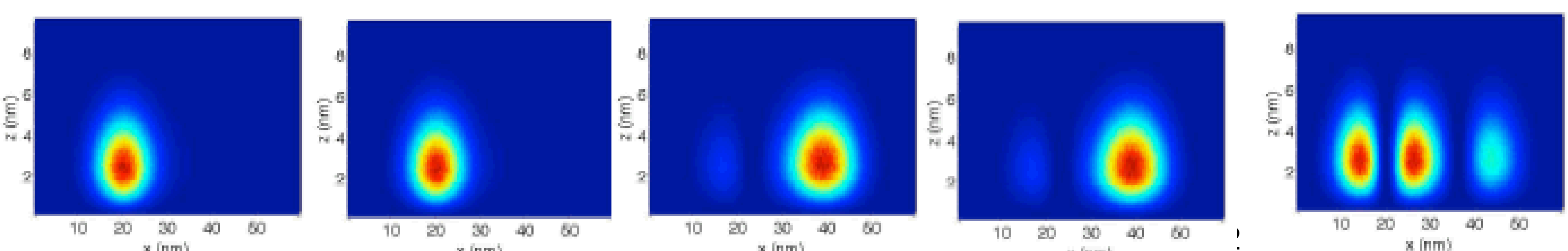


Defect at center of one dot (1e states)

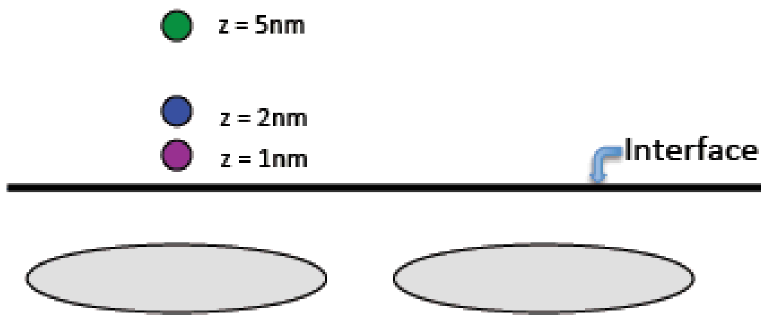






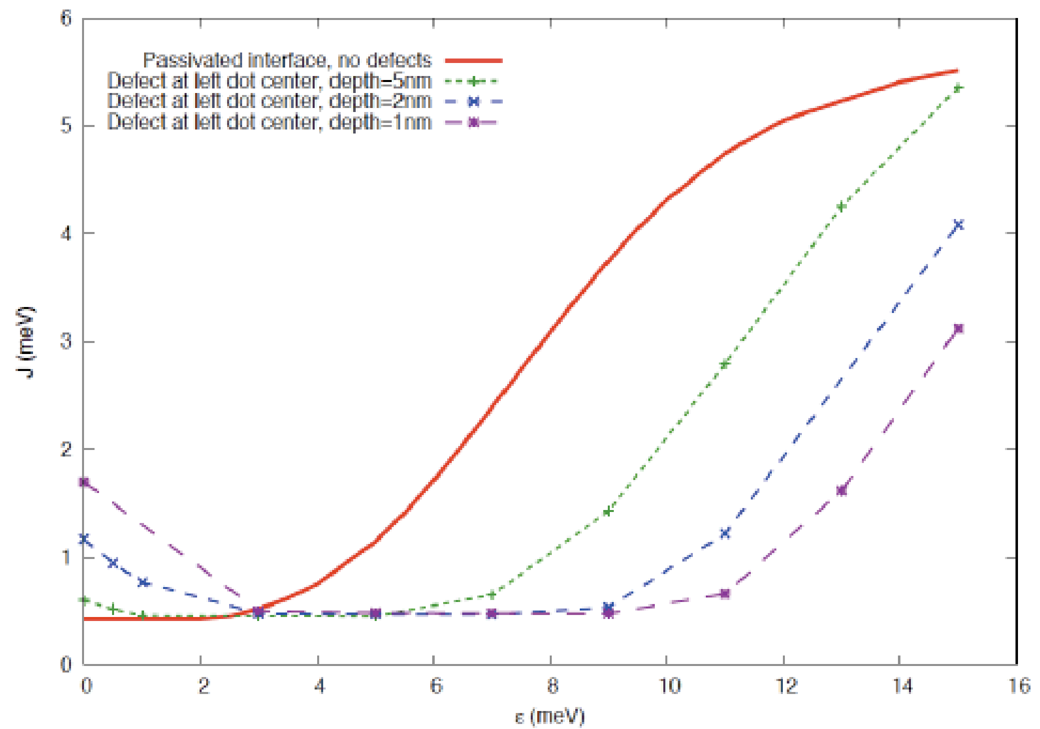


Defect at dot center

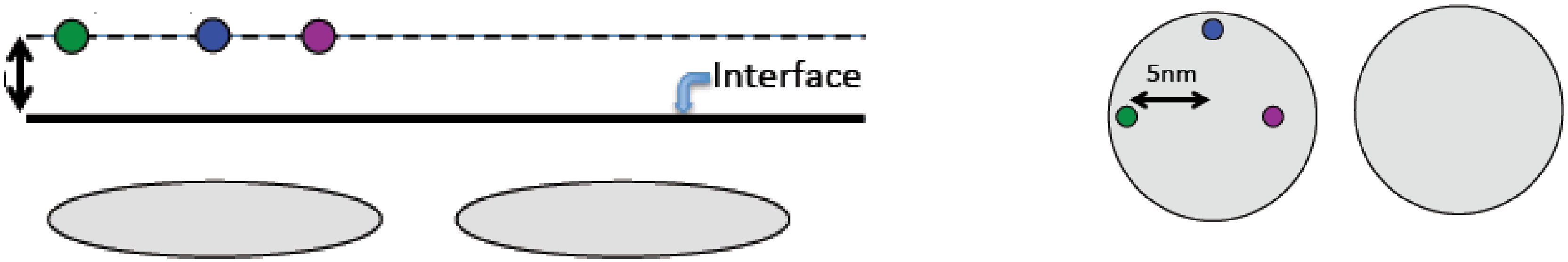


• Defect away from the tunnel barrier manifests as a shift in the J-curve (modified detuning)

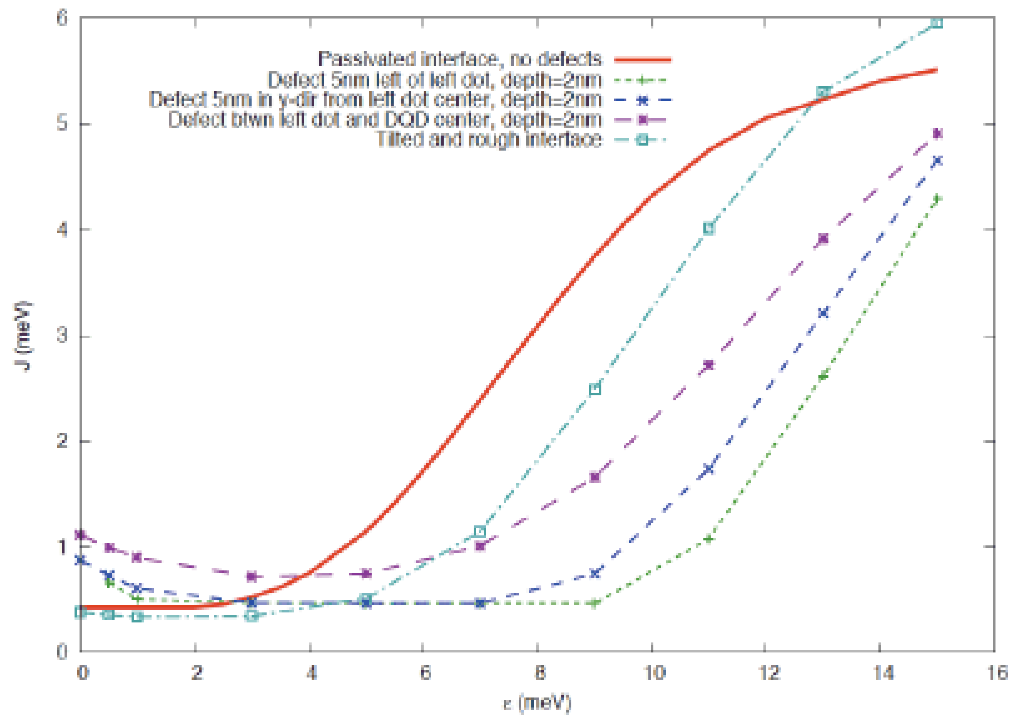
• Produces asymmetry between the (0,2) and (2,0) occupation by changing the electrostatic landscape.



Defect at different distances from barrier

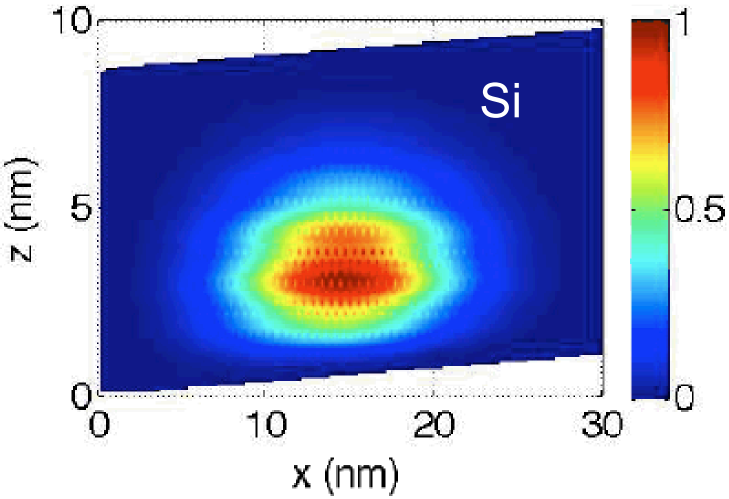


• J-curve is sensitive to defect location relative to the dots

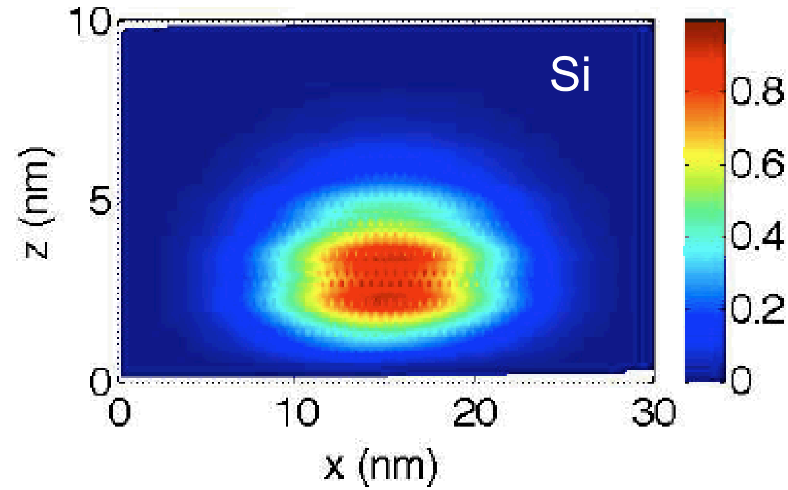


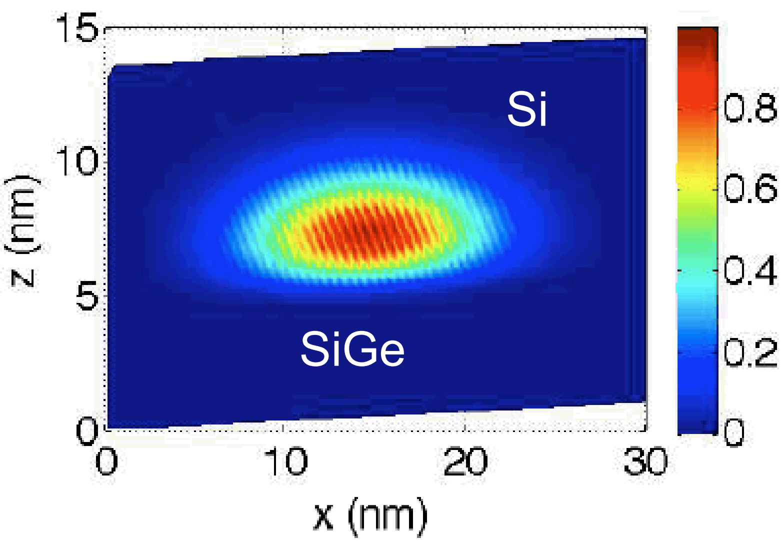
Atomistic models of interfaces: miscuts + alloy disorder

2 degrees (step length 3.8 nm, 7:1/4)



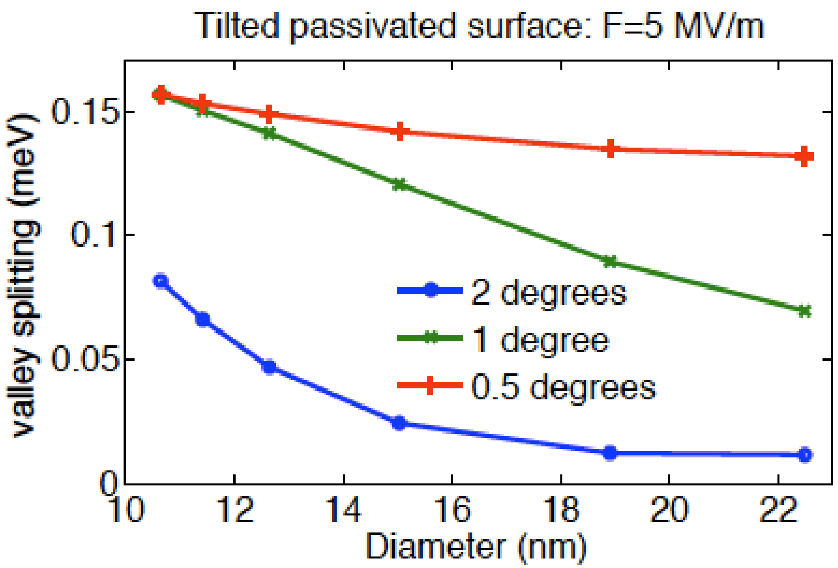
0.5 degrees (step length 15 nm, 28:1/4)

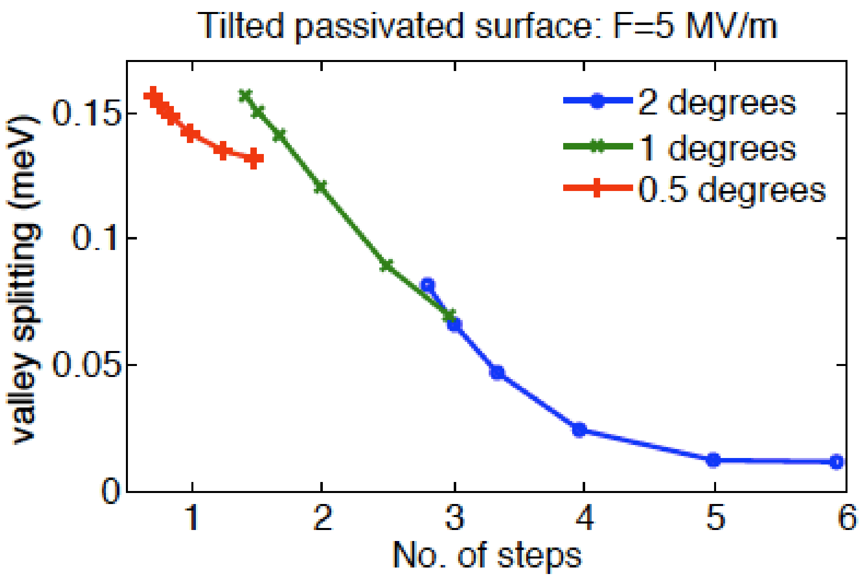




- QDs parabolic in x, y
- Uniform E-field in z (5-10 MV/m)
- 20% Ge, 80% Si
- Kharche et. al., APL 90, 092109 (2007)

Effect of tilt / ideal steps





Higher tilt suppresses VS.

At fixed tilt, larger dots -> smaller VS

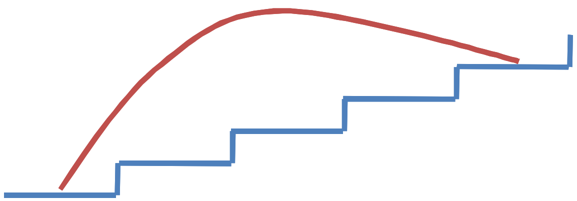
VS -> number of steps the wf samples.

E-field increases VS.

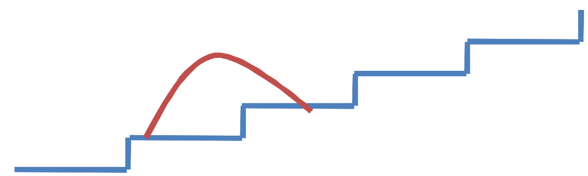
Intuition from EMT

M. Friesen et al., APL 89, 202106 (2006)

Extended wavefunction



More confined wavefunction



Step height: a0/4 (monolayer)

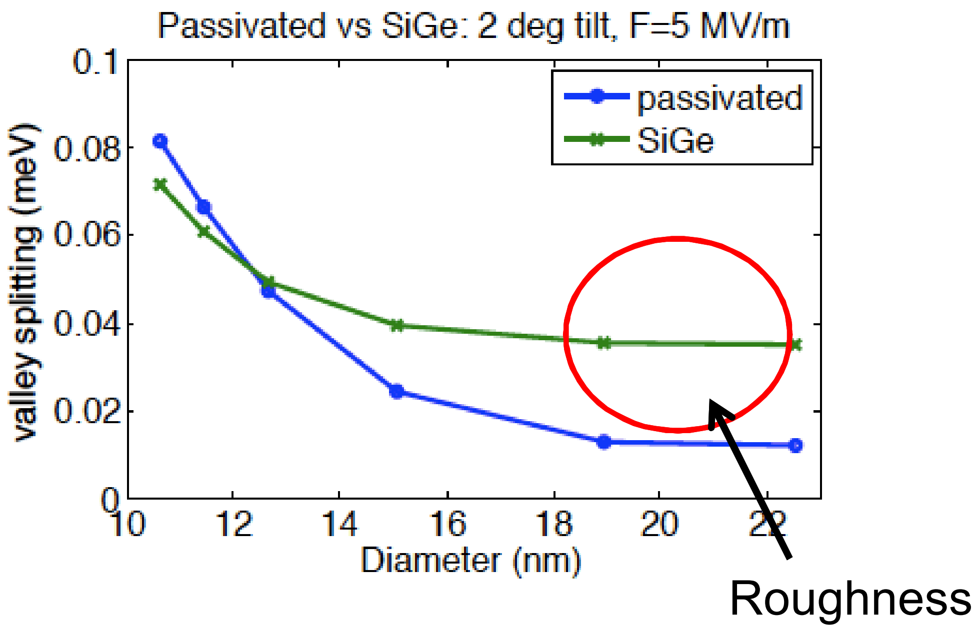
VS: $$E_v = 2\left| \int dr^3 e^{-i2k_0 z} \left|F(r)\right|^2 V_v(r) \right|$$

Ideal Steps: $z = \dfrac{a_0}{4}$ $\qquad 2k_0 z = 0.85\pi$

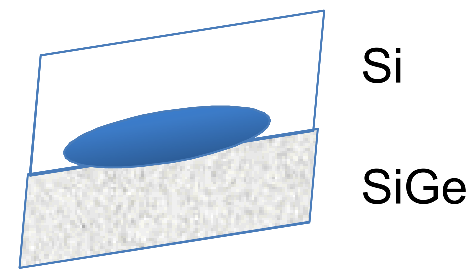
Roughness randomizes the phase factor, cancels out the suppression.

Effect of barrier material (alloy disorder)

Passivated vs. SiGe barriers



2 degree tilt

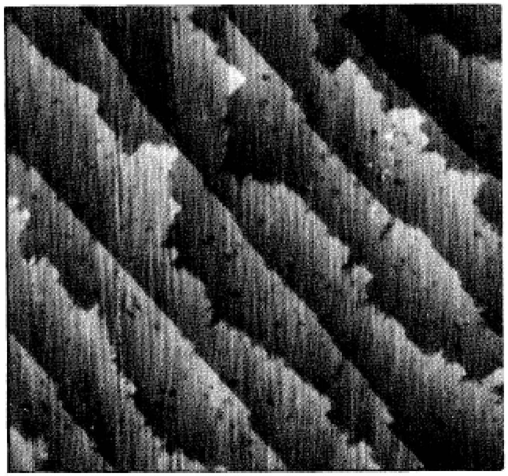


Alloy disorder -> atomistic fluctuations in CB edge.

Less quantum confinement -> less VS.

Roughness -> increases VS (tends to nullify tilt).

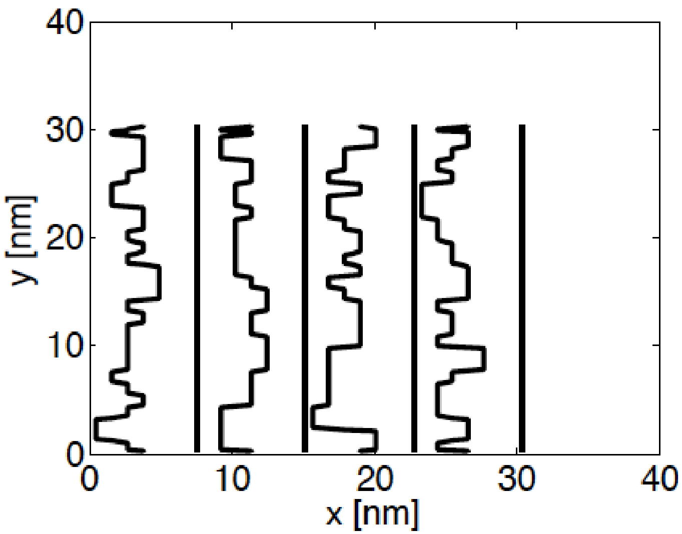
Atomistic models of interfaces: step roughness

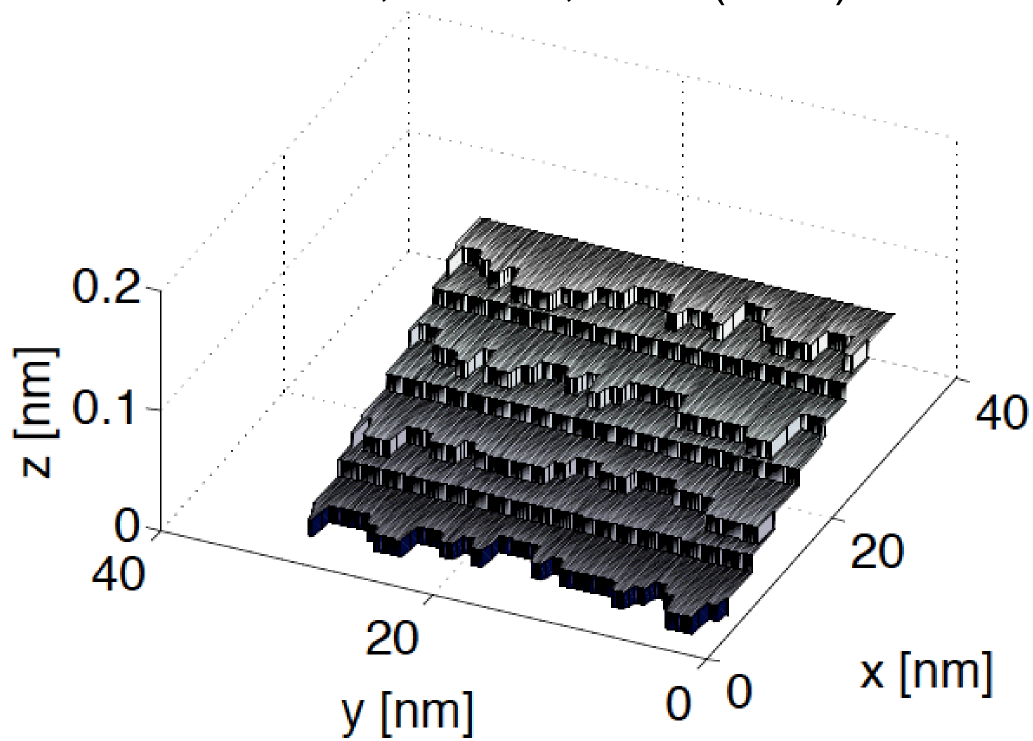


Roughness model: alternate ideal and rough steps, Zandvliet & Elswijk, PRB 48, 14269 (1993).

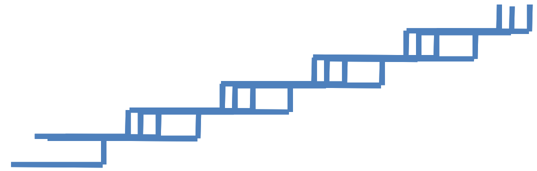
Other models:
Goodnick et al.,PRB 32, 8171 (1985)
Jones et. al., PRL 75, 1570 (1995)

Reconstructed surfaces in y

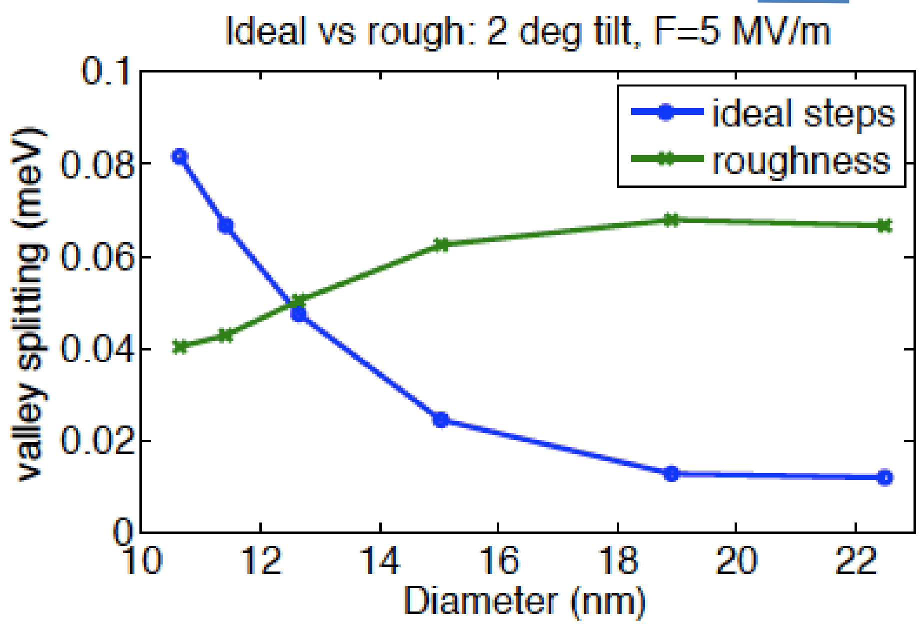




Effect of step roughness

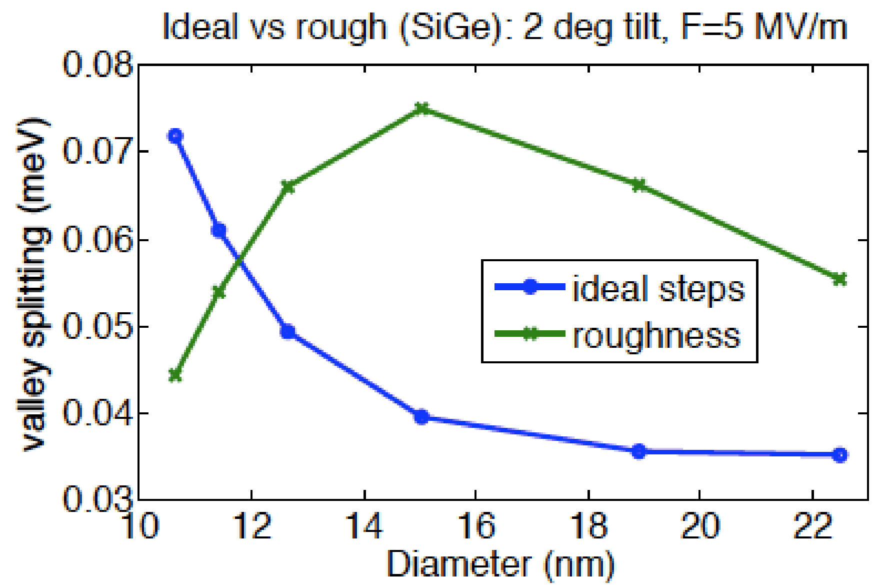


Passivated



2 degrees

SiGe



2 degrees

Roughness increases VS: partially cancels the effect of tilt.

Alloy disordered systems are more complicated.

Future work: Different roughness profiles

Conclusions

• Atomistc tight-binding – a high precision tool for device modeling

• Hyperfine Stark effect modeling is helping to understand measurements

• Developed TB + CI methodology to investigate J-curves

• J-curves are sensitive to defect locations and densities, but mostly tunable

• Effect of valley splitting, surface roughness, miscuts can be studied