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Atomistic simulations of valley splitting in silicon quantum dots in the presence of disorder

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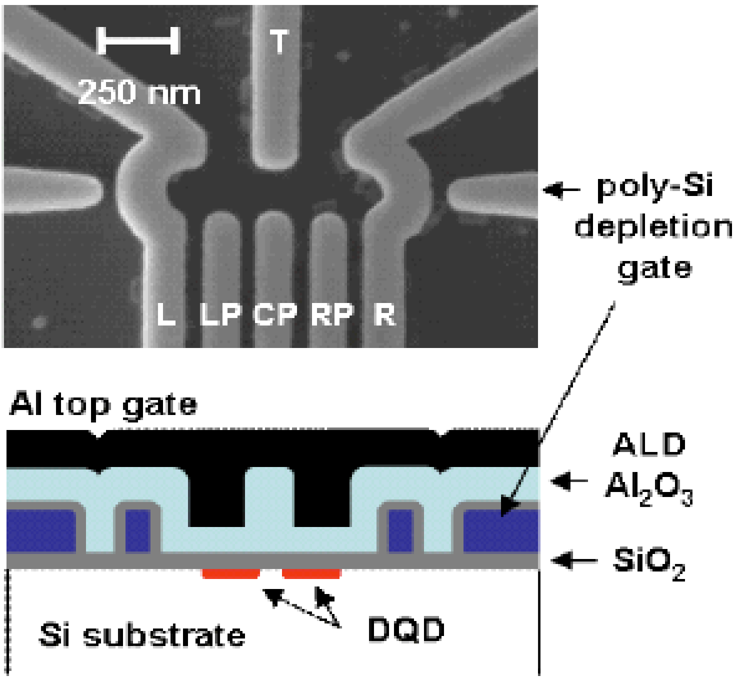
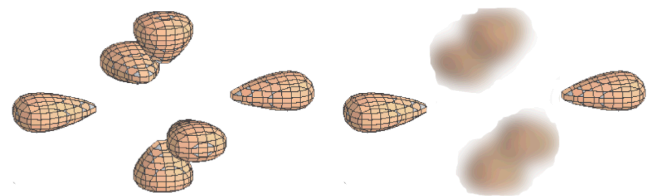
Valley splitting in Si QDs

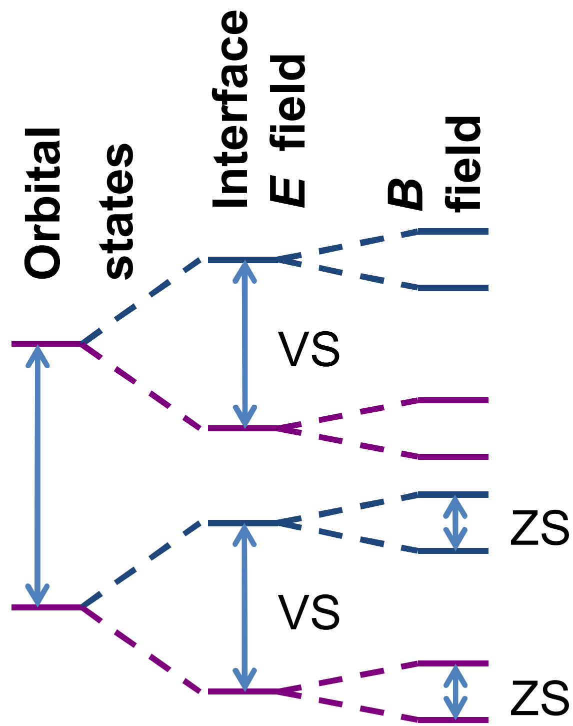
SNL QIST: DQD S-T Qubits in Si



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

Conduction band valleys in Si





Outline

1. Valley Splitting in SQD:

- Miscut (Tilt / Ideal steps)
- E-field
- Barrier material (alloy disorder + strain)
- Surface roughness

Method: Atomistic tight-binding (NEMO 3D)

2. Valley Splitting in DQD:

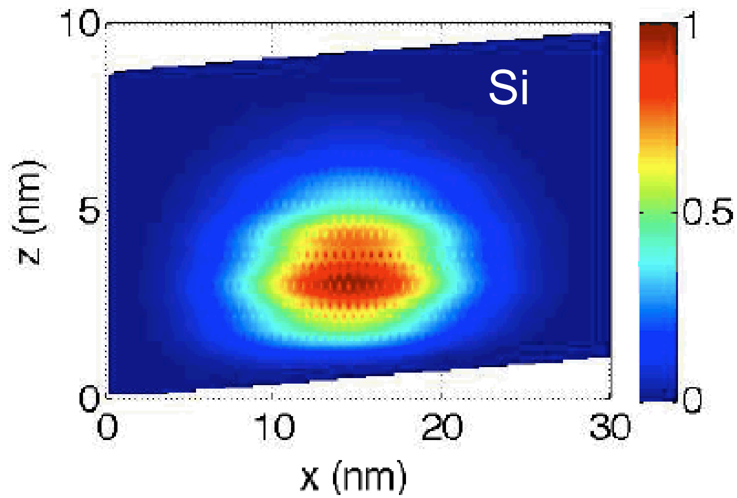
- 2e states with fields, tilt

Method: Tight-binding (NEMO 3D) + Full Configuration Interaction

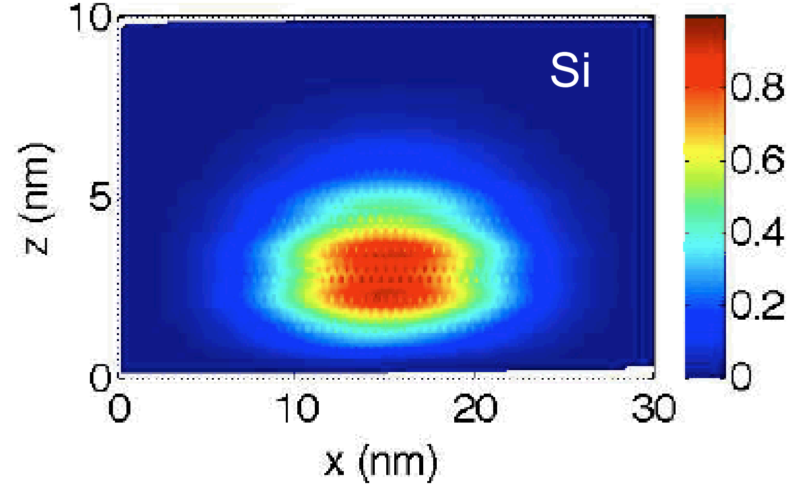
(Thanks to Erik Nielsen)

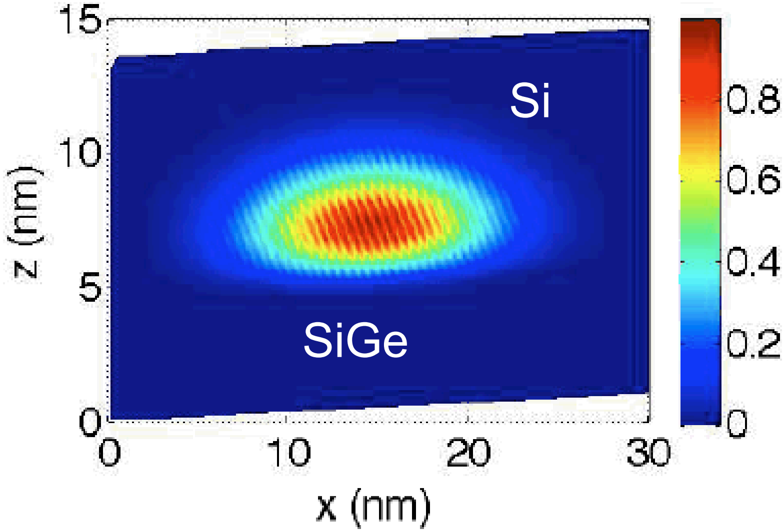
Atomistic models of interfaces : Miscuts

2 degrees (step length 3.8 nm)



0.5 degrees (step length 15 nm)





- 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)

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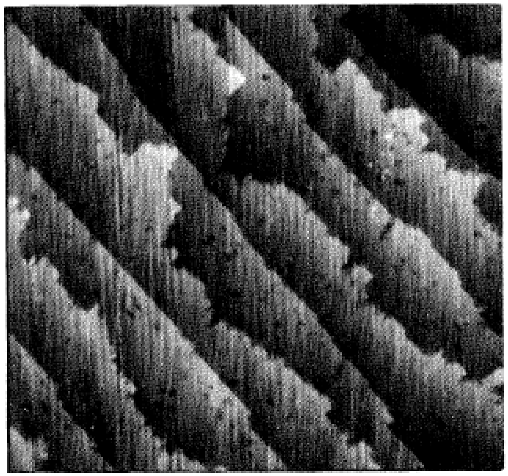
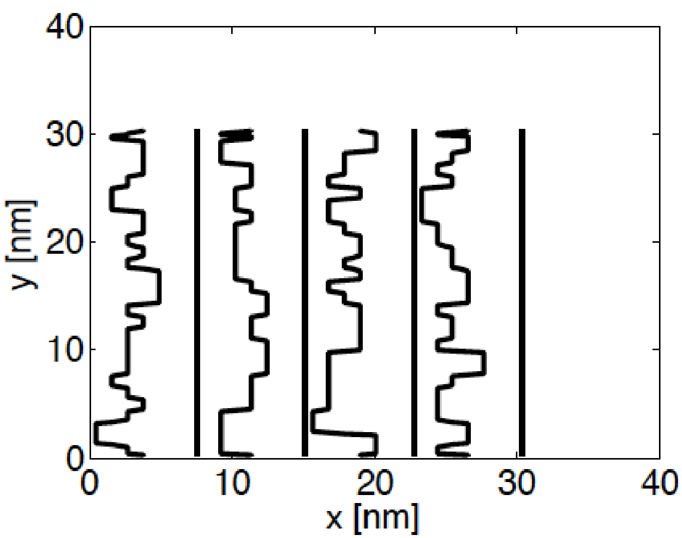
Atomistic models of interfaces: roughness

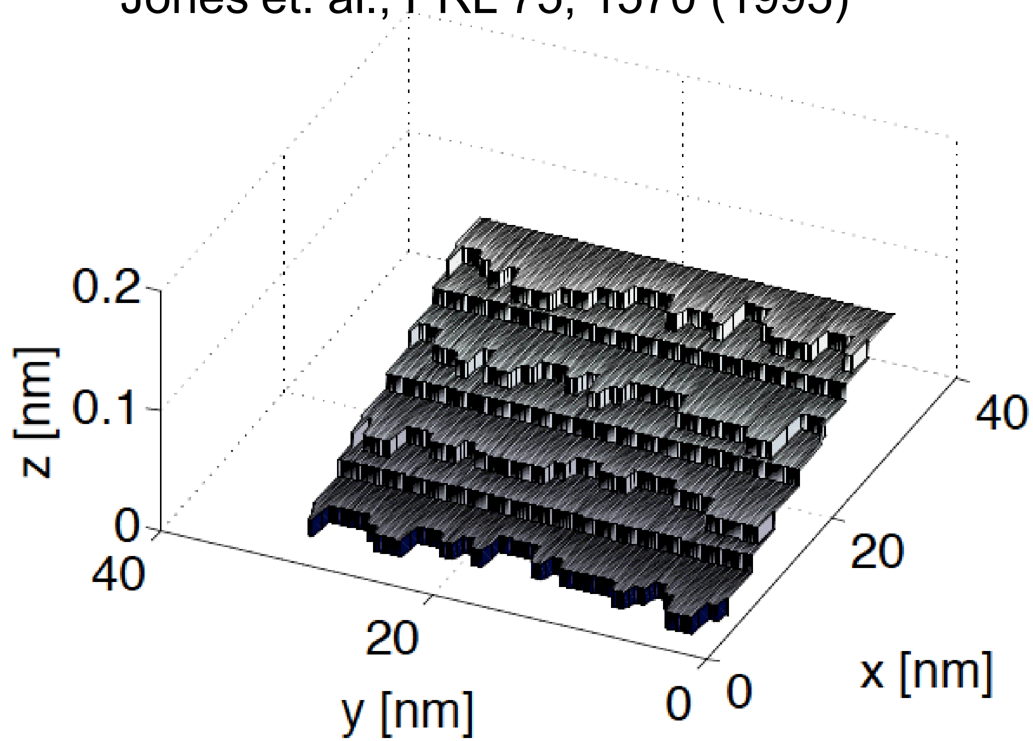


Roughness model: alternate ideal and rough steps, Zandvliet & Elswijk, PRB 48, 14269 (1993).

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

Reconstructed surfaces in y





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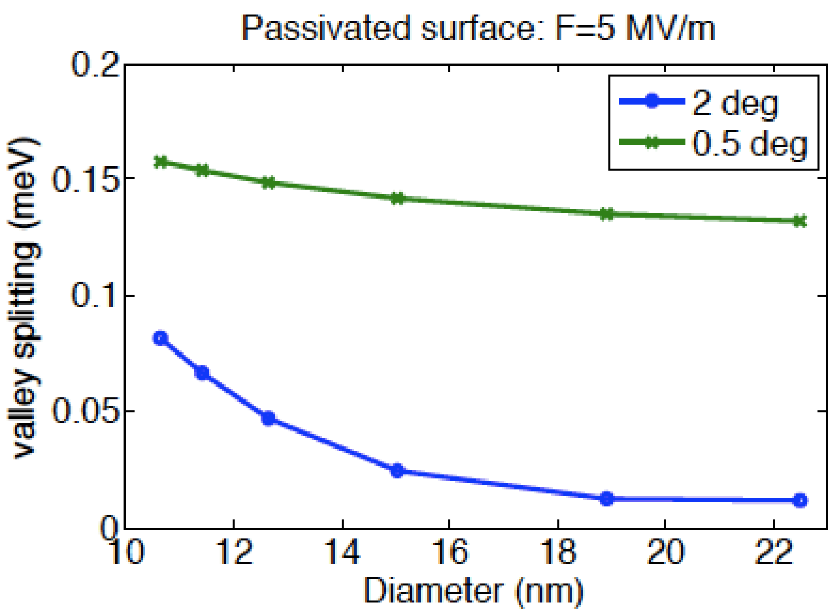
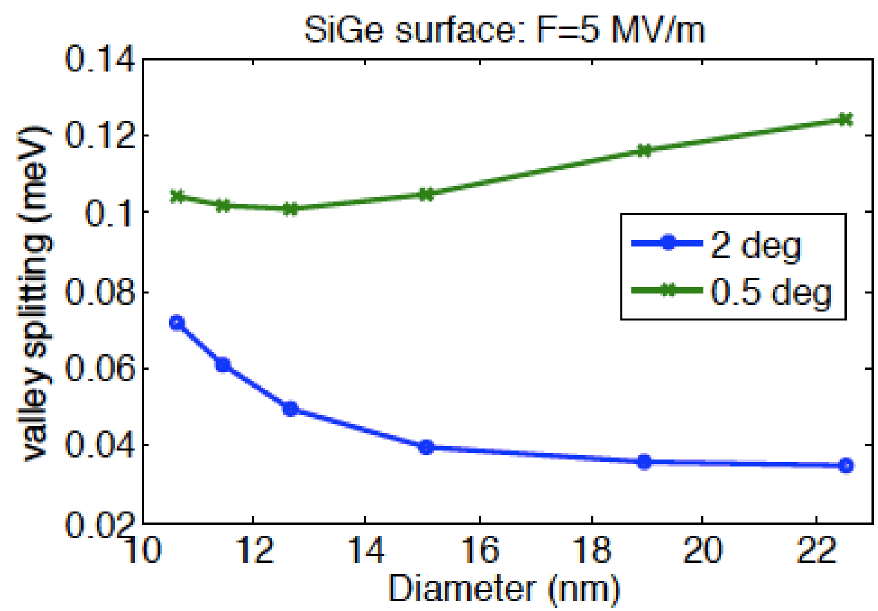
Effect of tilt



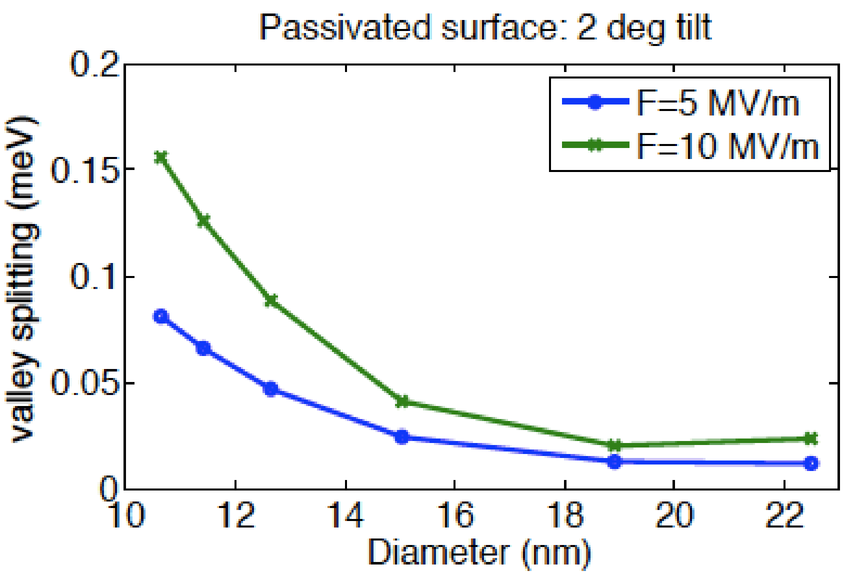


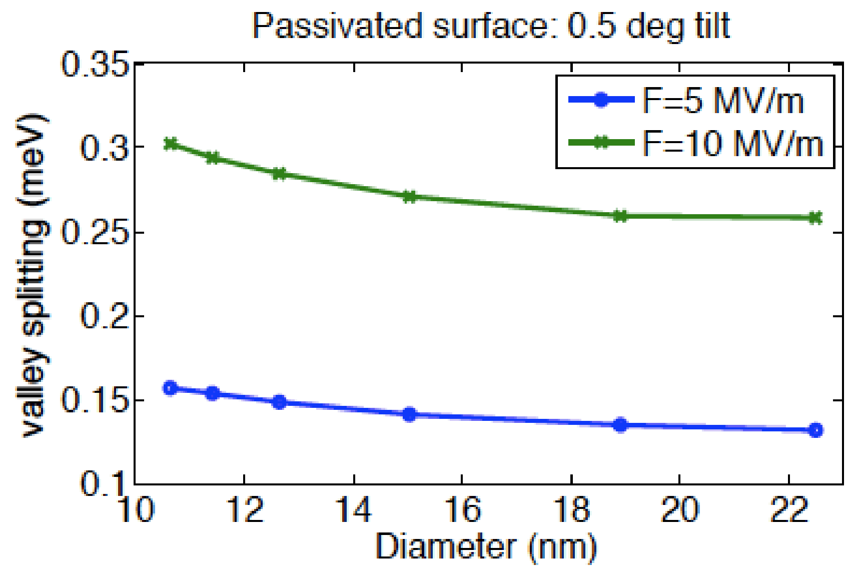
Higher tilt suppresses VS.

Larger dots experience smaller VS with tilt.

Alloy disorder at the interface plays a role

Effect of E-field



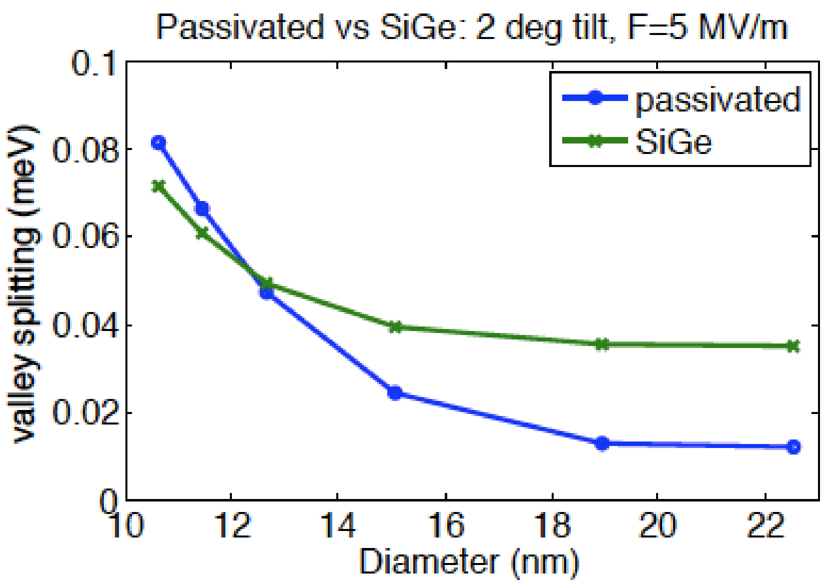


Higher vertical E-fields produce higher VS irrespective of tilt or disorder.

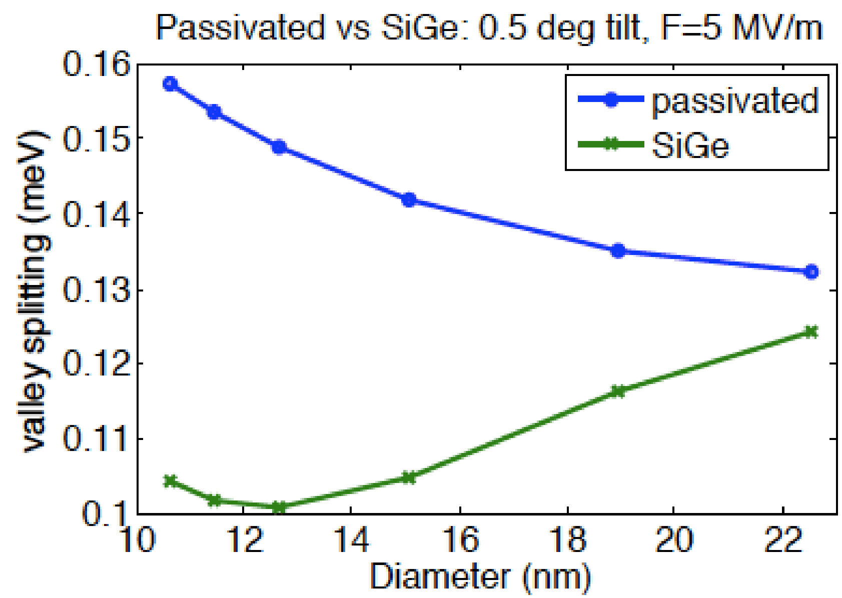
Holds in SiGe-Si dots also.

Effect of barrier material

Passivated vs. SiGe



2 degree tilt

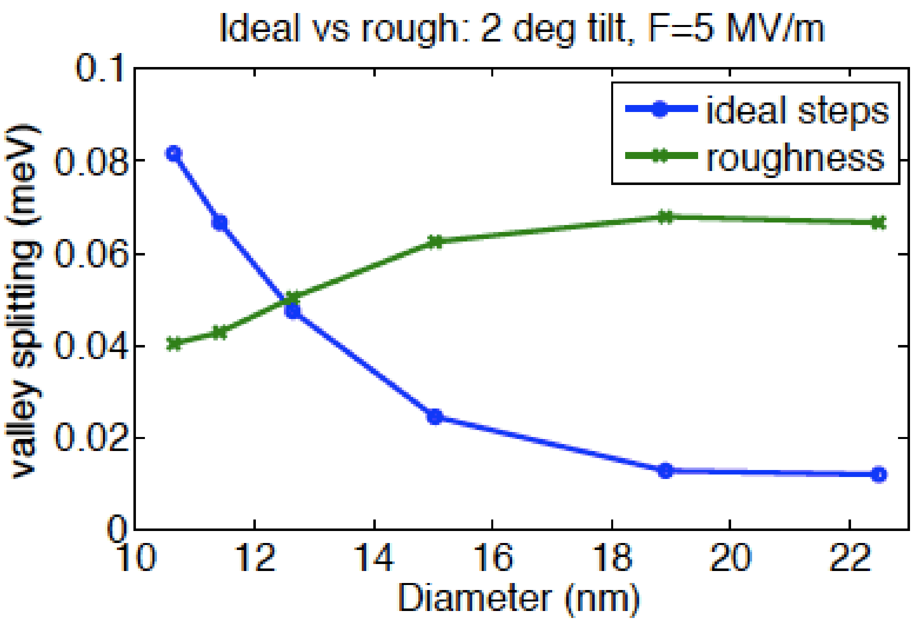


0.5 degree tilt

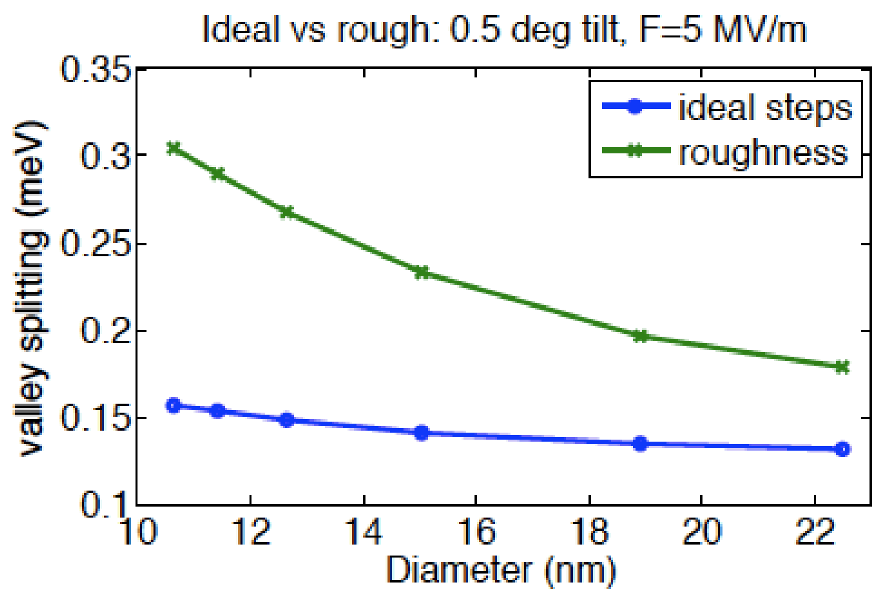
Alloy disorder introduces atomistic roughness in CB edge.

Effect of roughness

Role of step roughness in passivated surfaces



2 degrees



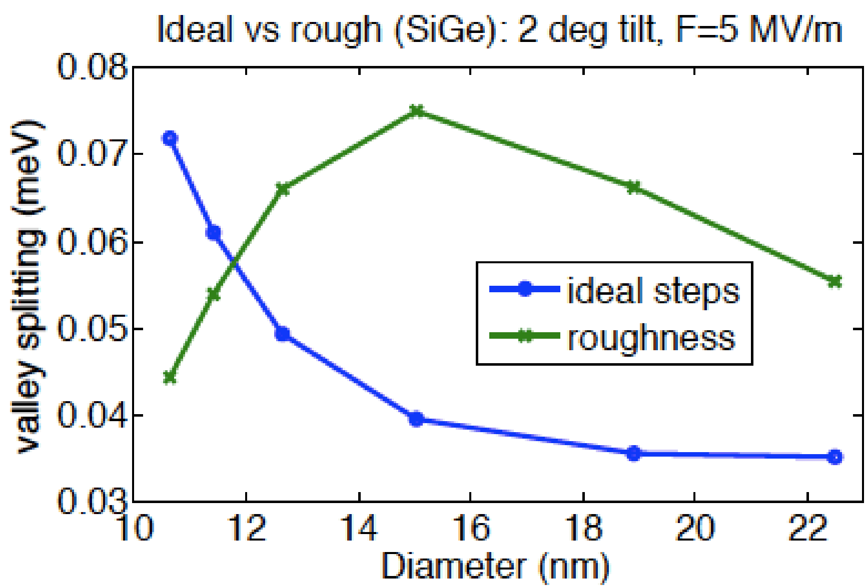
0.5 degrees

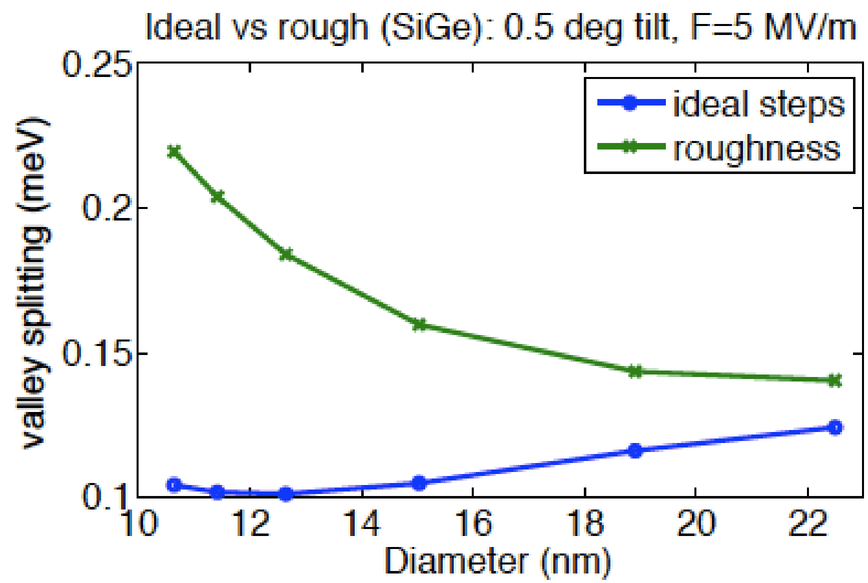
Roughness increases VS: Cancels the effect of tilt.

M. Friesen et. al., APL 89, 202106 (2007).

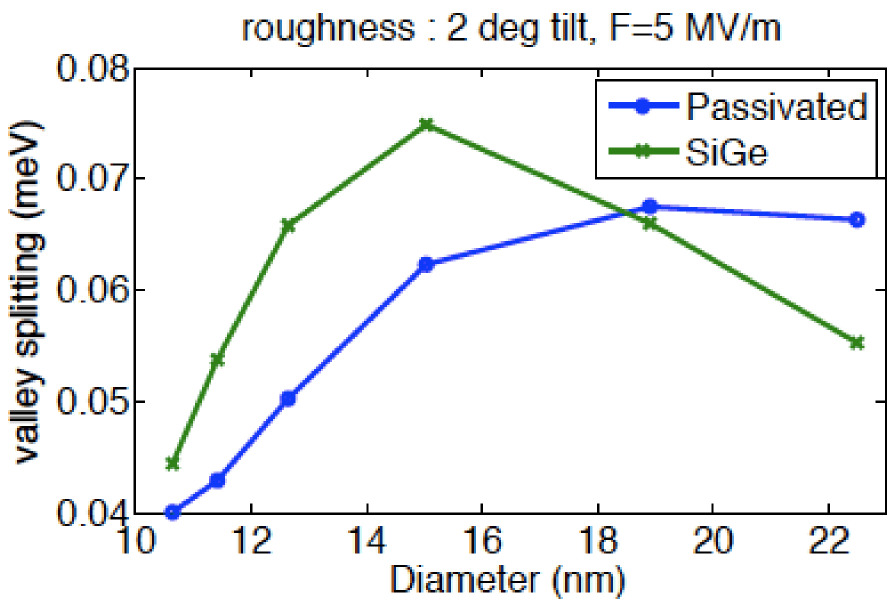
Step roughness + alloy disorder

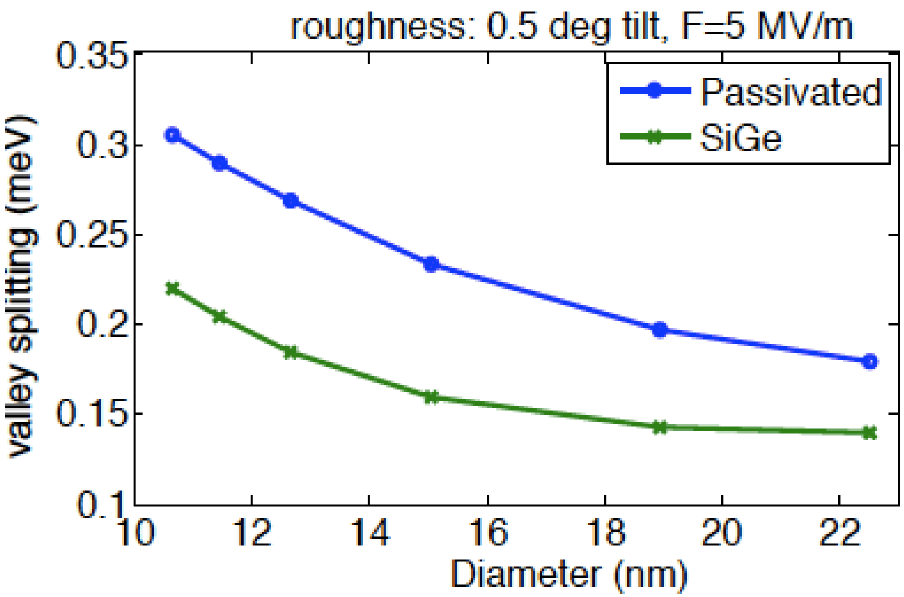
SiGe barriers





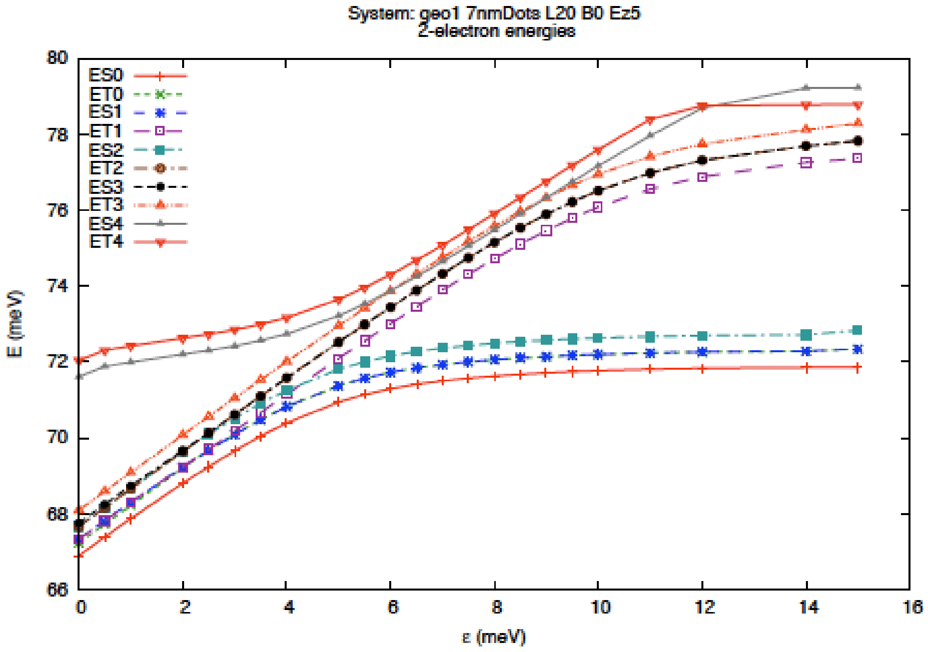
Role of alloy disorder

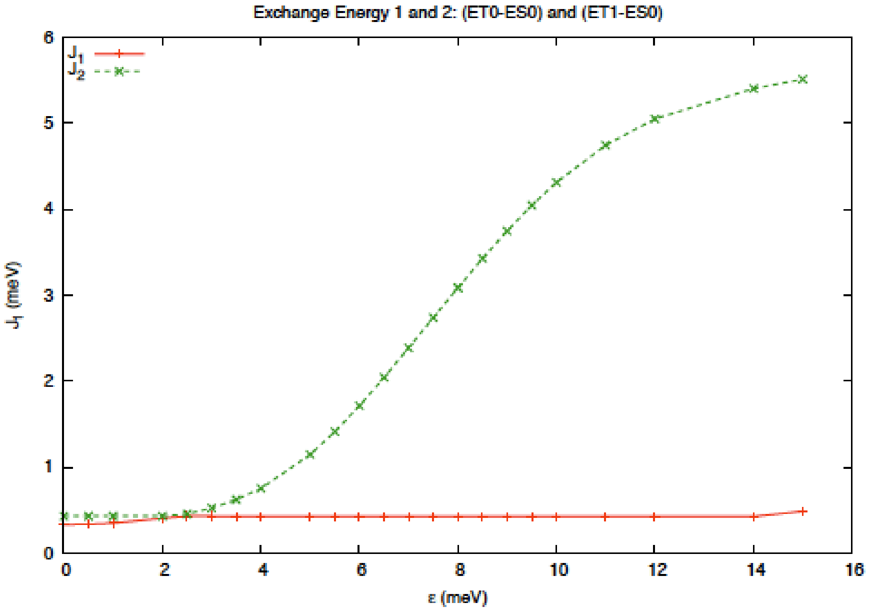




DQD 2e states with small VS

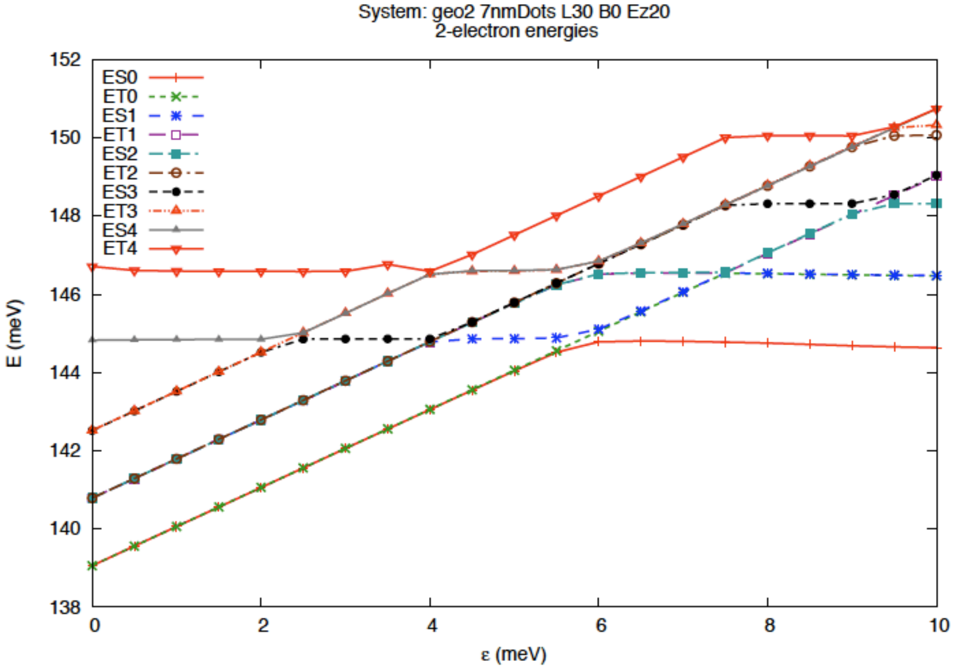
F=5 MV/m

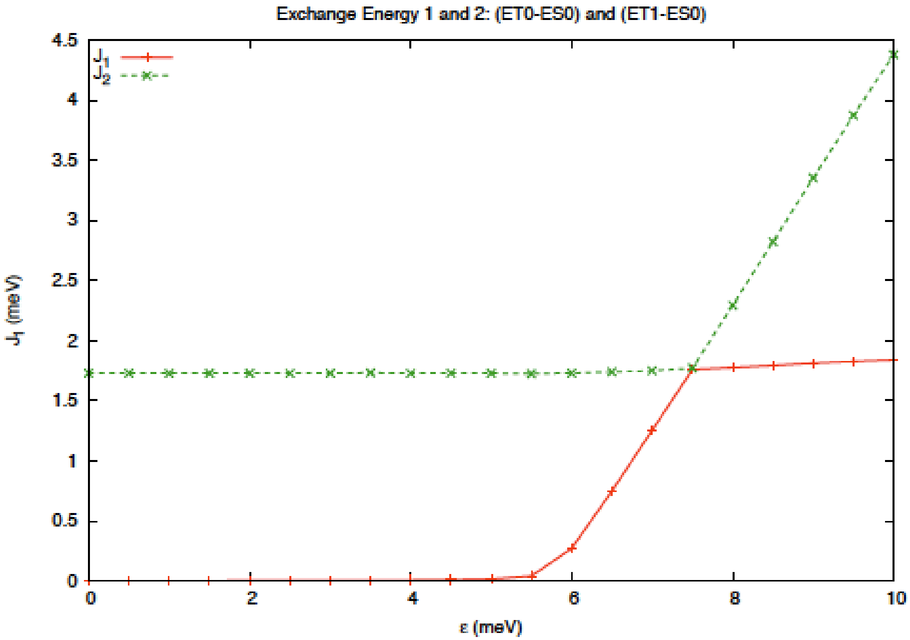




DQD 2e states with large VS

F=20 MV/m





Conclusions

- Tilted lattice suppresses VS in Si QDs
- Step roughness reduces the suppression
- E-fields increase the magnitude of VS
- Barrier material and alloy disorder are important
- TB + CI combined to obtain 2e states of a multi-valley Si DQD
- Effect of VS shown on the exchange splitting