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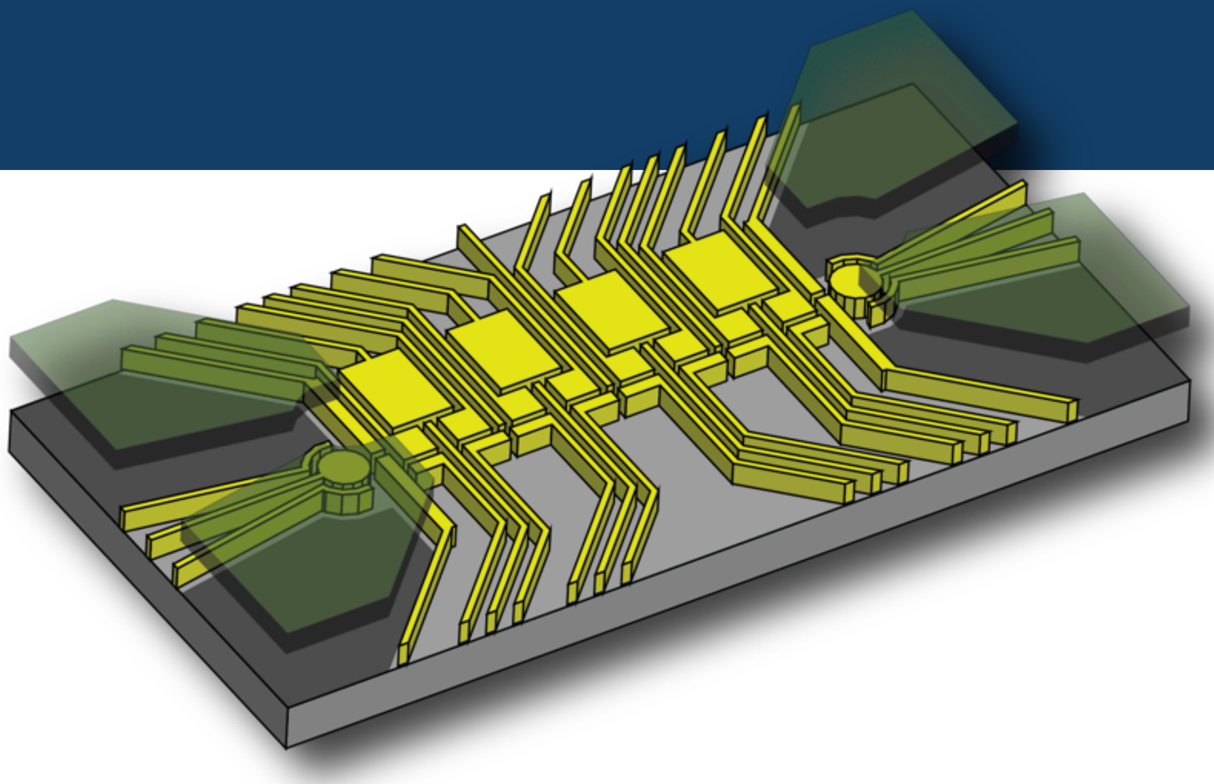

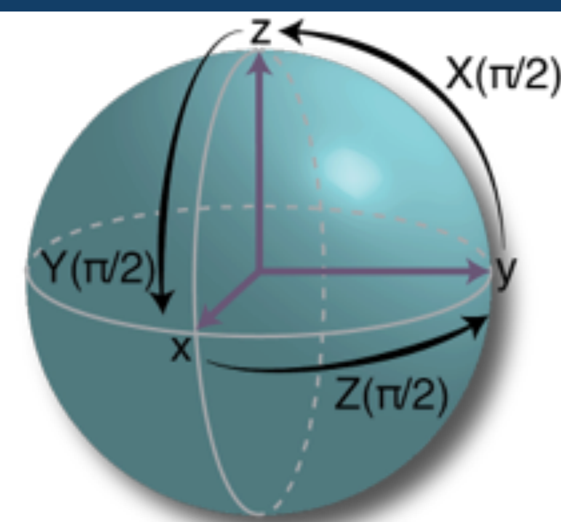

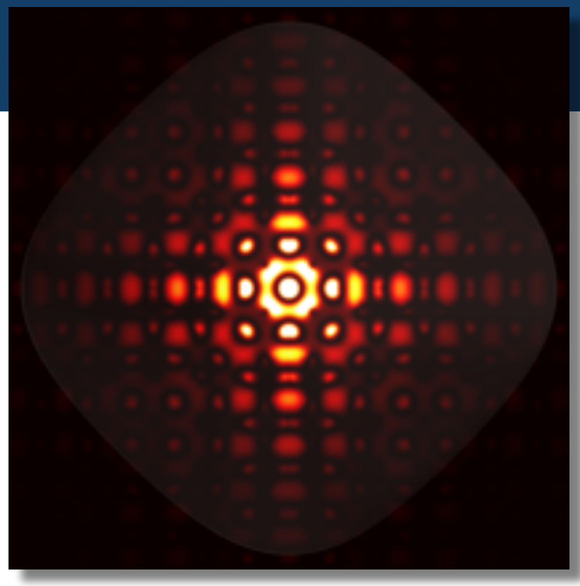

Computational modeling of semiconductor qubits

John King Gamble

Center for Computing Research, Sandia National Laboratories

CCR
Center for Computing Research

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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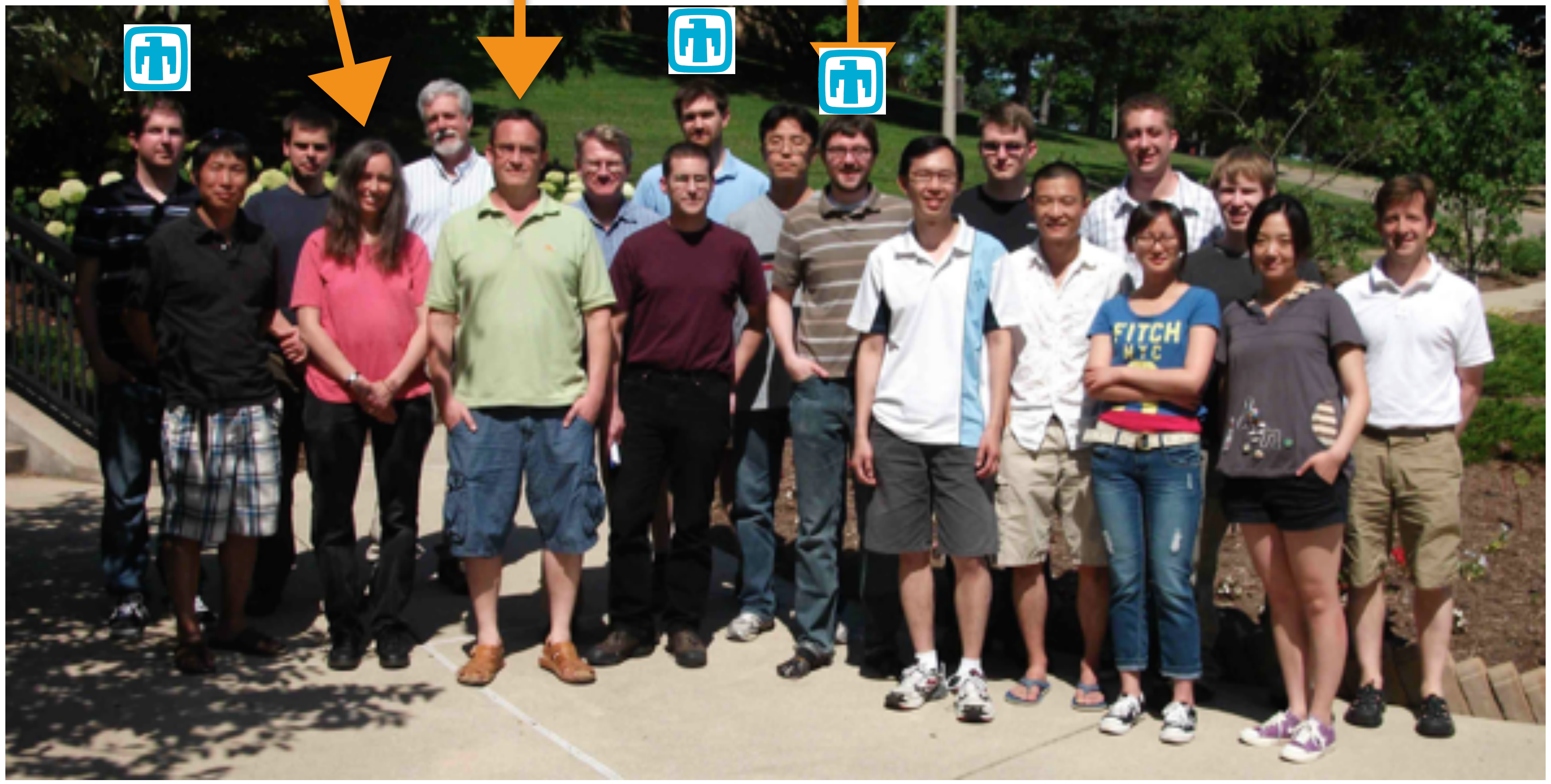
Rewind four years…

- PhD from UW in 2013
  - Supervisors: Sue Coppersmith and Mark Friesen
- Moved to Sandia National Labs as a Truman Fellow 2013-2016.
- Permanent staff at Sandia 2016-present.

- Toward the end of my PhD, we started digging into the physical details of Si qubits that had been previously swept under the rug.
- I proposed to extend my graduate work in a Truman Fellowship at Sandia.
- This is the story of what happened over the next three years.

= WI folks we've "convinced" to come to Sandia :)

Sue Mark F. me

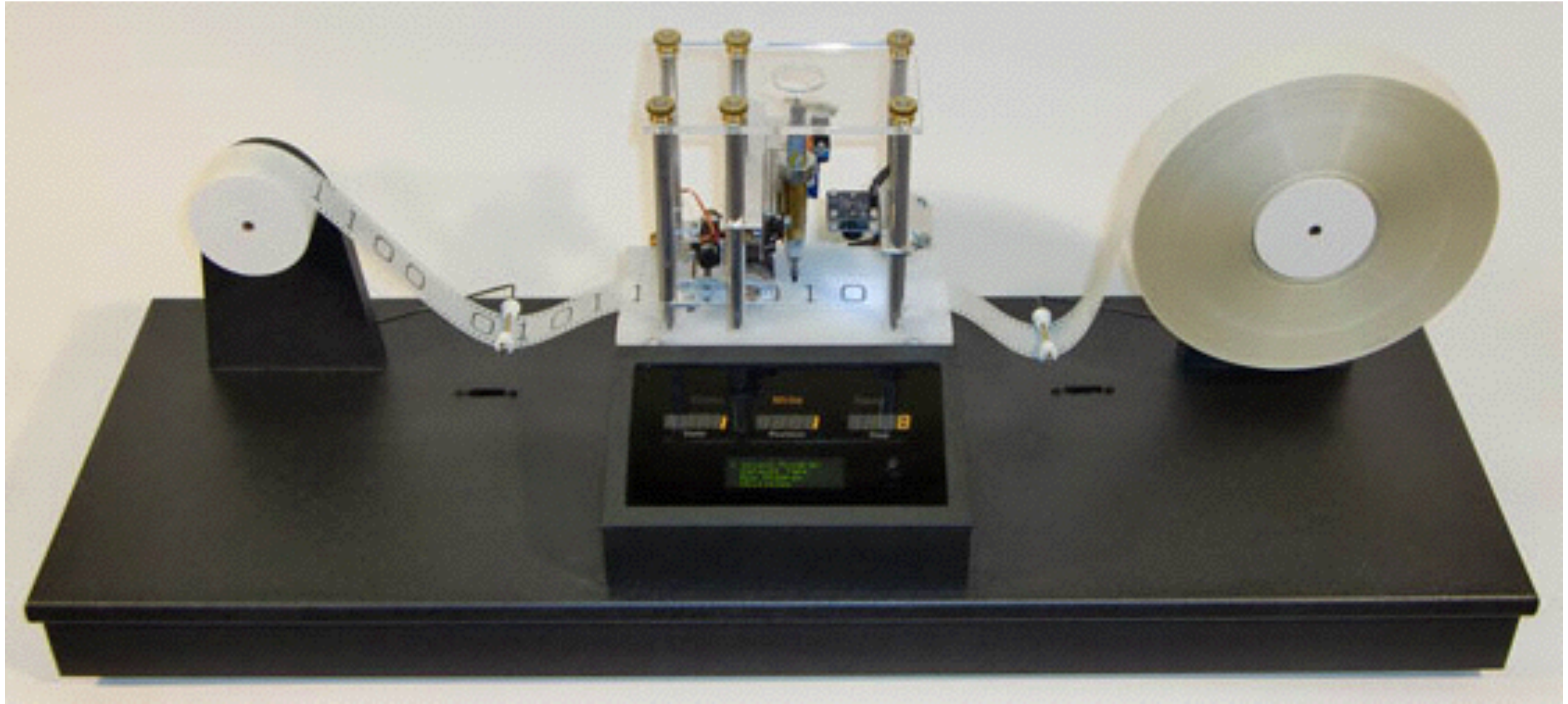


UW Si qubit group circa 2010.

Let's talk about information

- What can you do with information?
  - Acquire
  - Process
  - Transmit
- Where does the information live?
  - Paper
  - Computers
  - Genetic code

- **Information is physical!!**



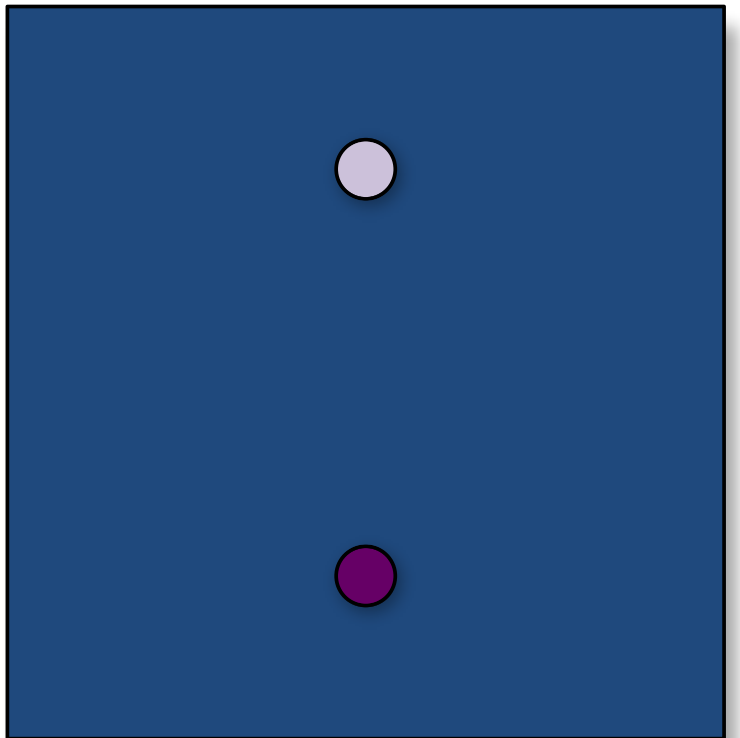
Example: physical Turing machine.

Question: How does my *choice* of physical system in which information is stored affect my ability to *acquire, process,* and *transmit* it?

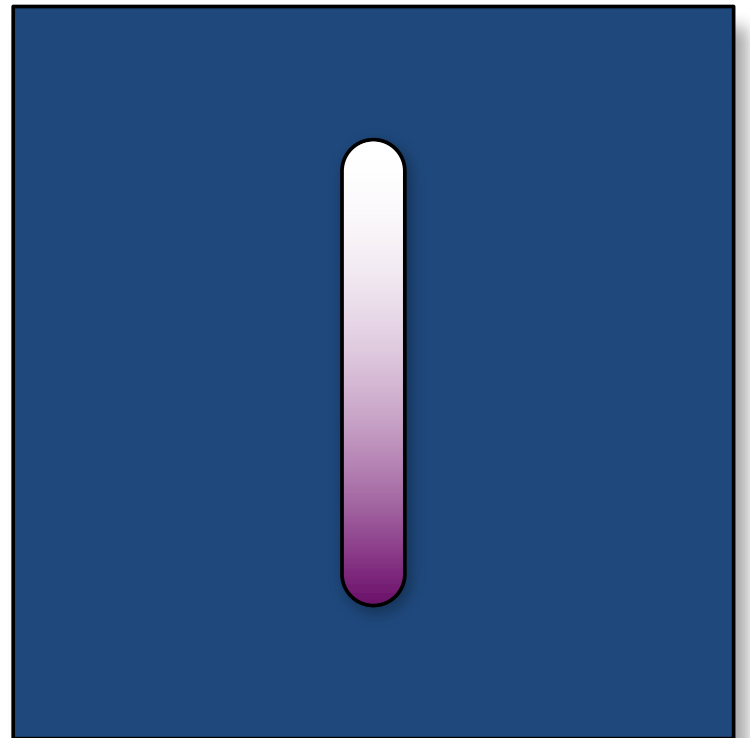
Answer: It can have a profound effect!

How information is stored in a physical system

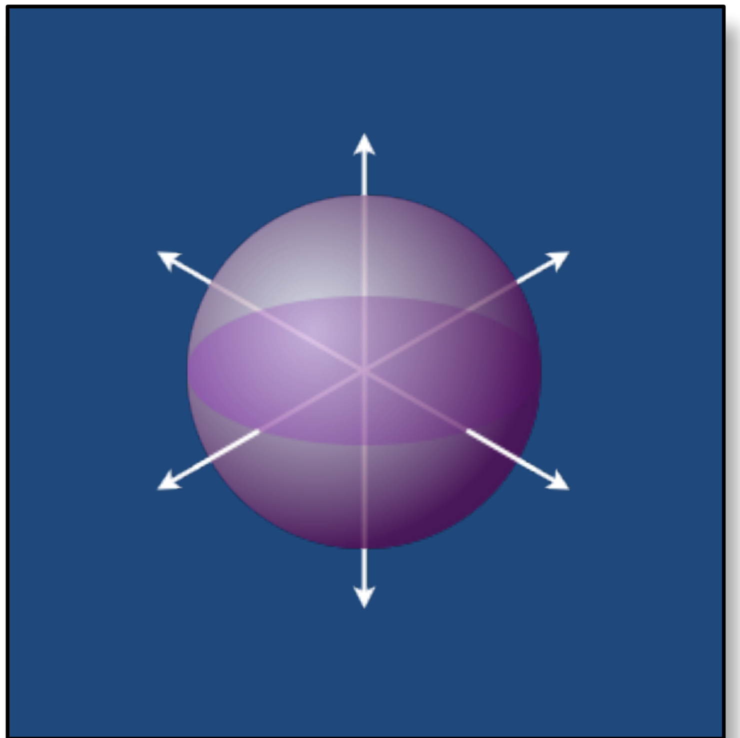
classical, deterministic



classical, probabilistic



quantum



Bit:

- "On" or "off."
- State can be represented by one of two points.

Pbit:

- *Probability* of "on" or "off."
- Probabilities sum to one.
- State can be represented by a point on a line segment.

Qubit:

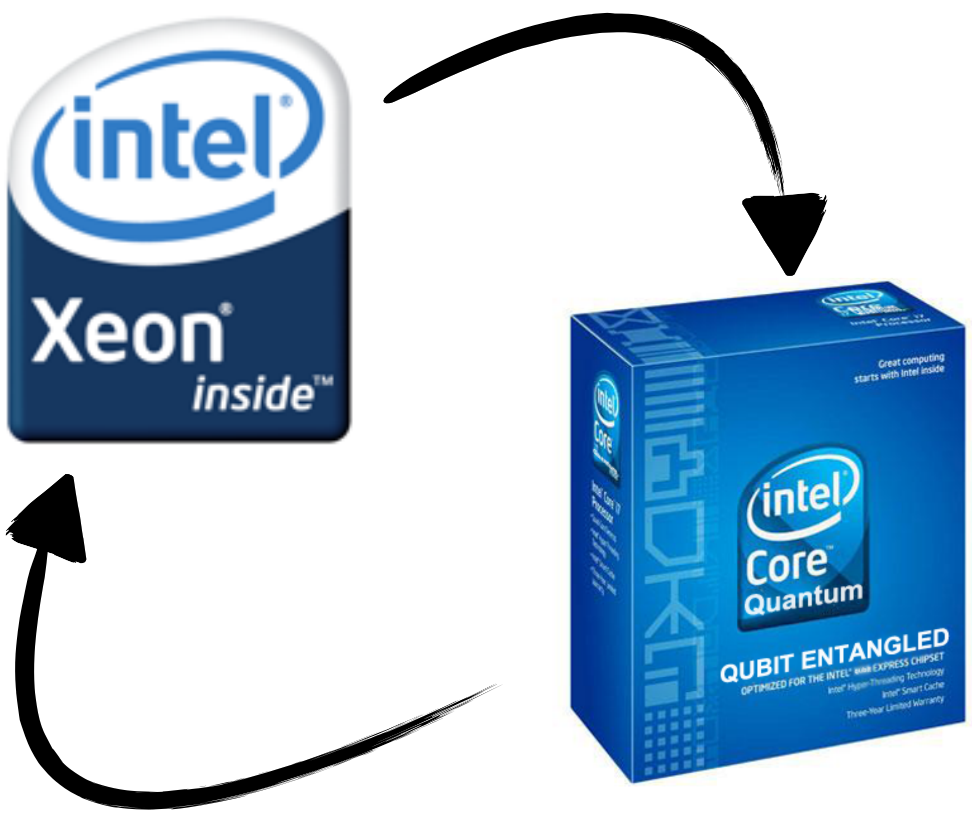
- *Amplitude* of "on" or "off."
- Probability is square of amplitude.
- Probabilities sum to one.
- State can be represented by a point on sphere.

What would a quantum computer be good for?

Shor's algorithm: exponential speedup for integer factoring.

Grover's algorithm: square root speedup for unstructured database search.

Not better for general-purpose computing: quantum co-processor



Quantum simulation (Feynman): Using a quantum computer to study physical systems directly (quantum chemistry, particle physics, condensed matter physics, etc.)

Examples of qubits

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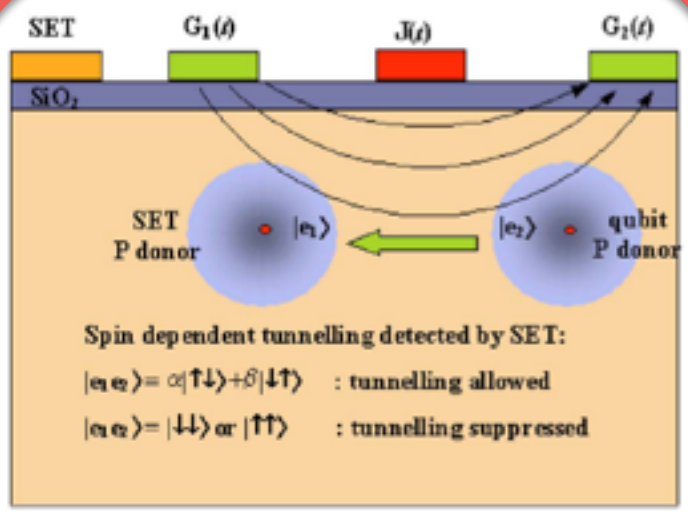
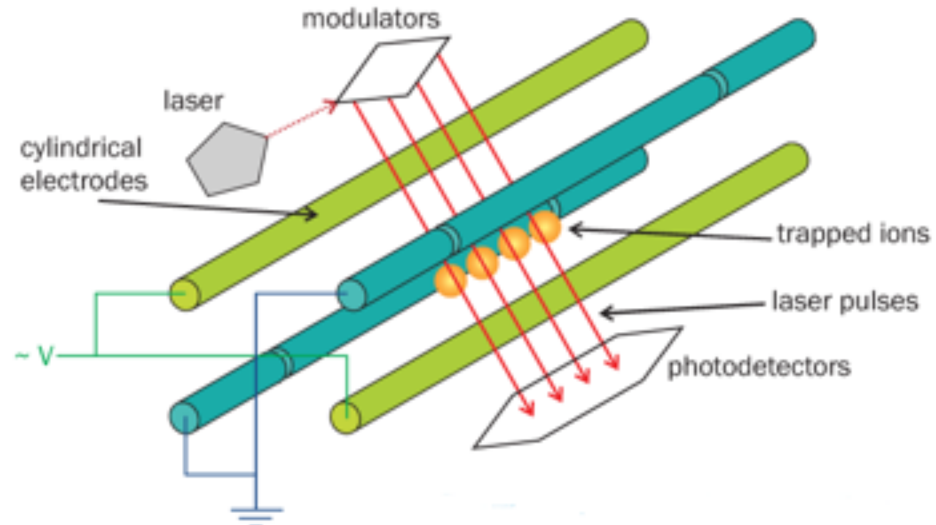
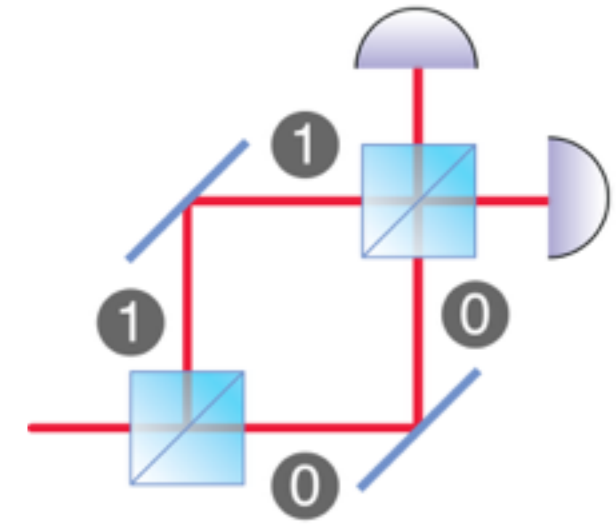


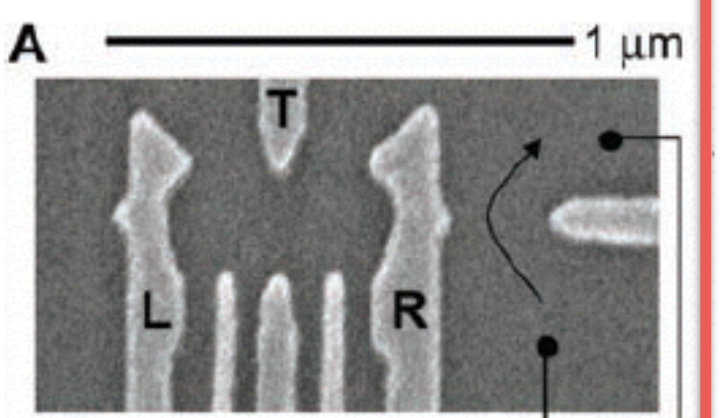
Semiconductor Donors



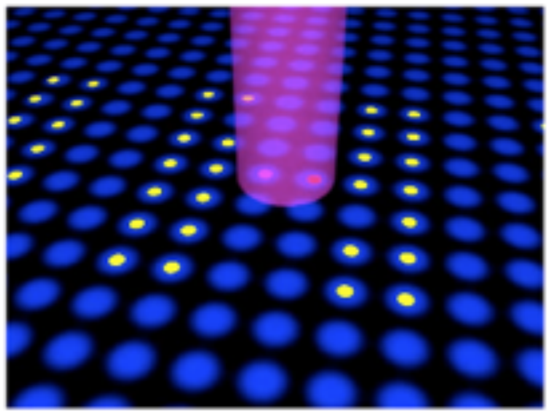
Trapped Ions



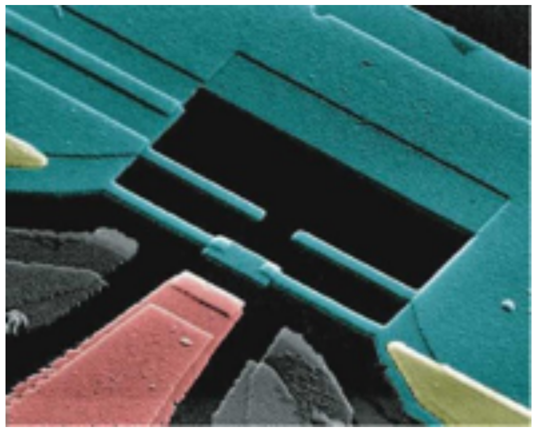
Optical



Semiconductor Dots

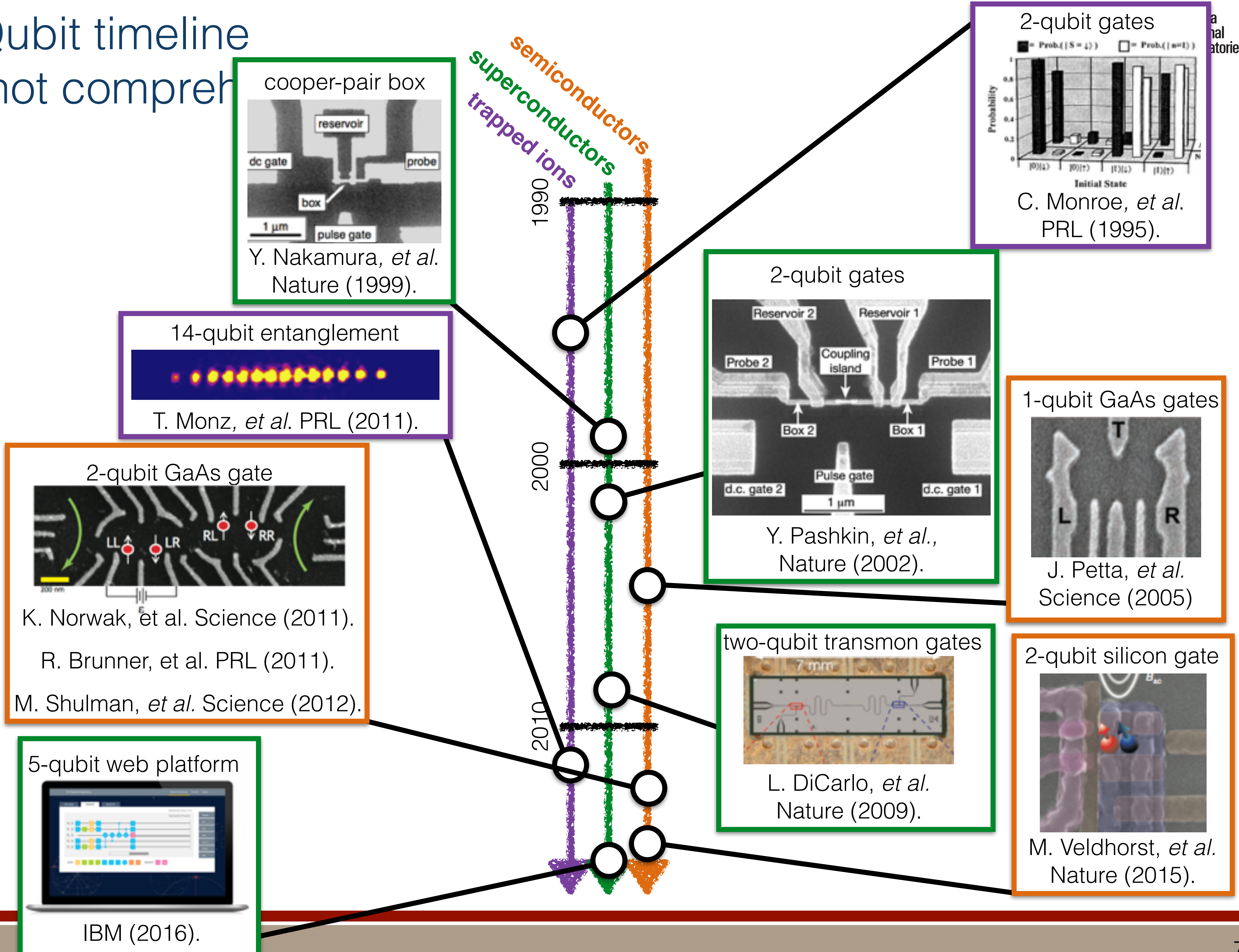


Trapped Atoms



Superconducting

Qubit timeline
(not compreh



Qubits in semiconductors: “artificial atoms”

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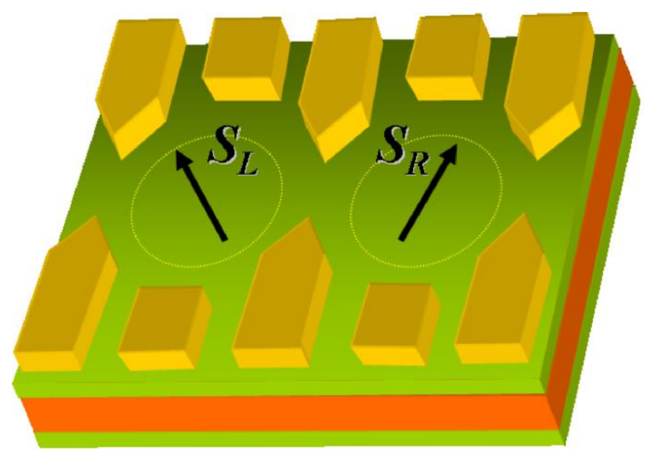
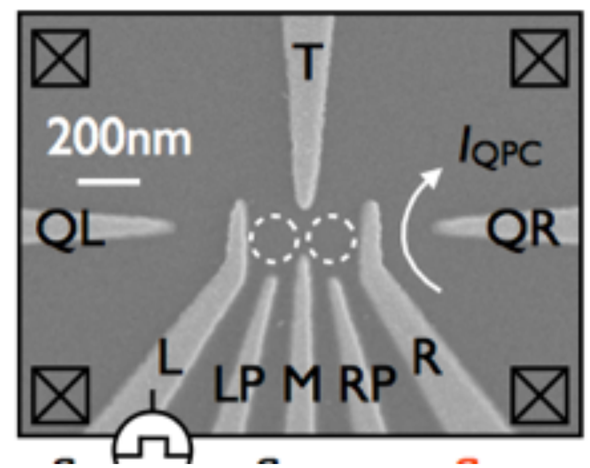
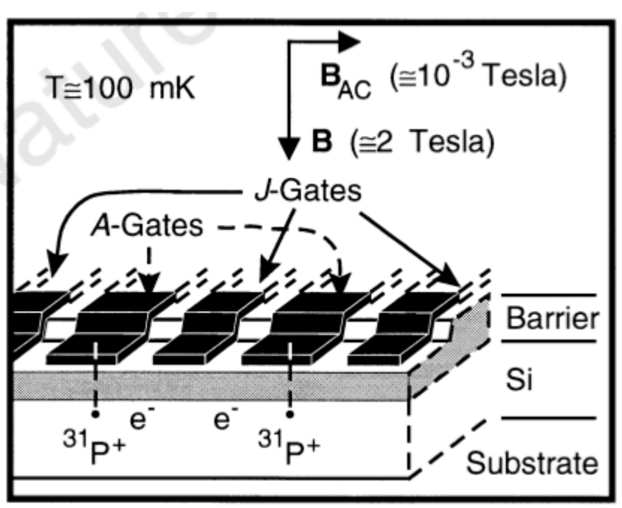
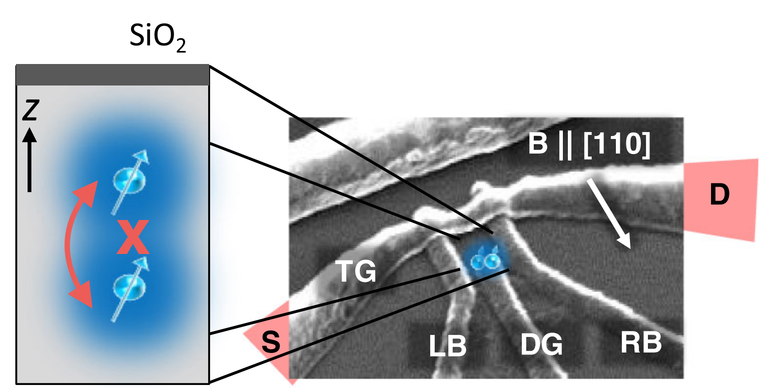
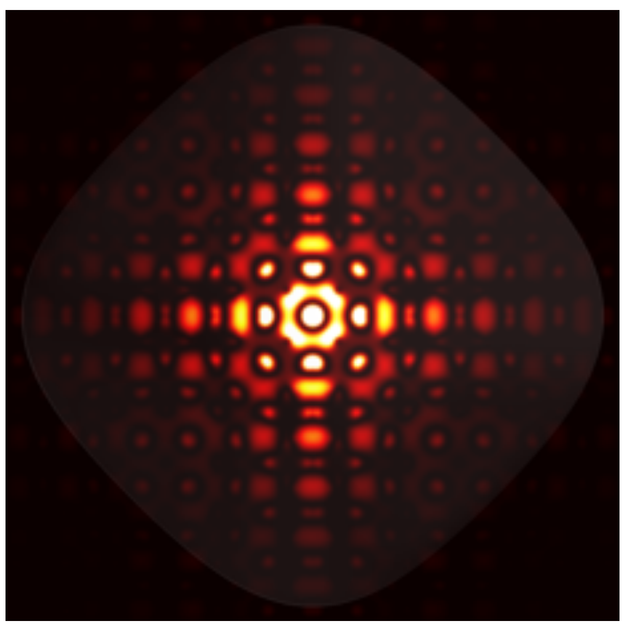
	Theoretical proposal	Example realization	Remarks
Electrostatic Quantum dots	 Loss & DiVencenzo, PRA (1998).	 [Kim, et al. Nature 511, 70 (2014)]	• Extremely flexible due to user-defined nanostructure. • Can achieve long-time coherence through materials engineering. • Risk: every dot is different.
Donor impurities	 Bruce Kane, Nature (1998).	 [Dehollain, et al. PRL 112, 236801 (2014)]	• Two qubits for the price of one (nuclear spin + bound electron spin)! • Nuclear spins have the highest fidelity of any known solid state qubit - every donor is (about) the same! • Risk: every donor-donor *coupling* is different.

Outline

Question: Donor qubits seem ideal from the standpoint of single-qubit operations, but can they be coupled reliably?

Answer: Not directly, but perhaps via dot-donor hybrid qubits. To be able to make predictions about this system, we need a theoretical framework that can handle *both* dots and donors!

Part 1:
donors are hard to couple directly



[Gamble & Jacobson, *et al.*, PRB **91**, 235318 (2015)]

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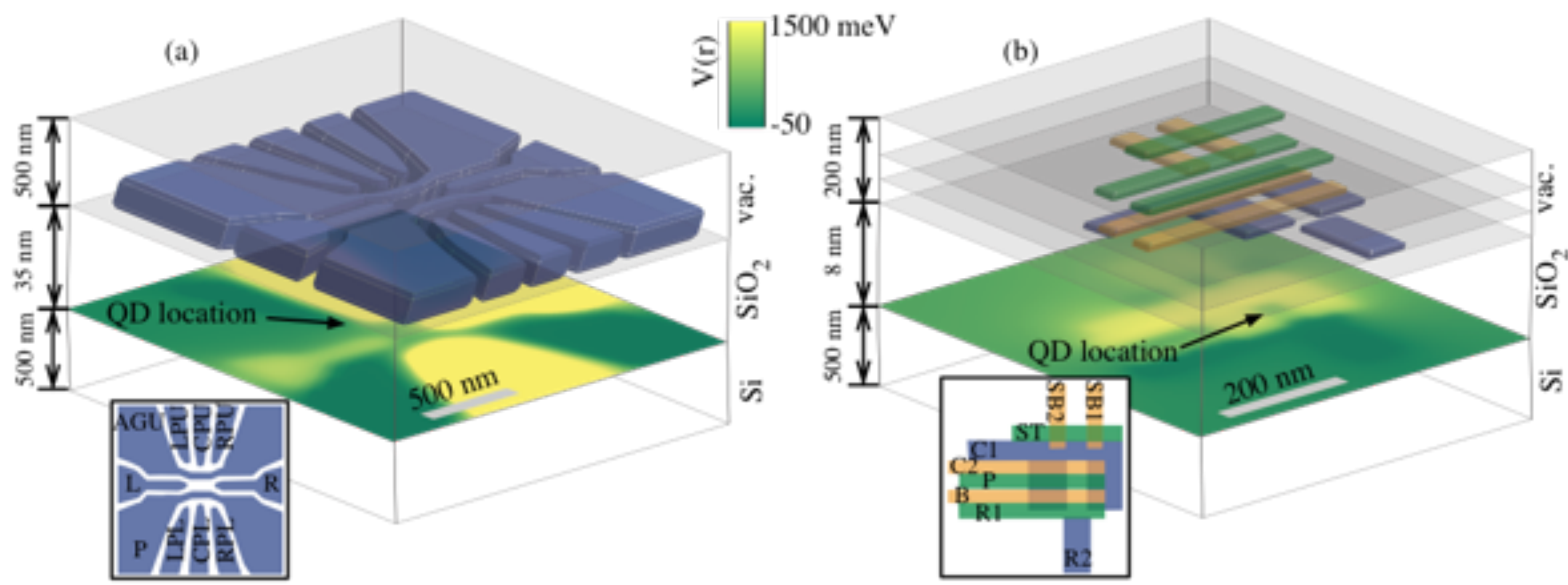
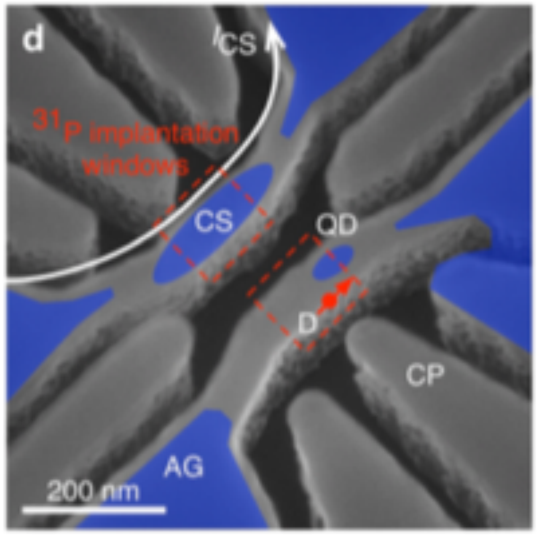


[Gamble, *et al.*, APL (2016)]

Combining both species of artificial atoms

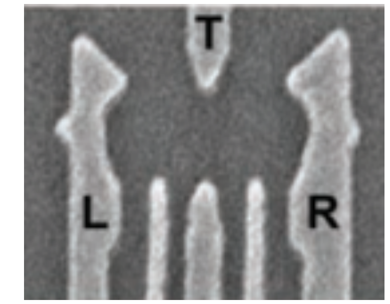


One cell has been demonstrated in experiment…

… and has been reproduced in M. Rudolph, *et al.* IEDM (2016).

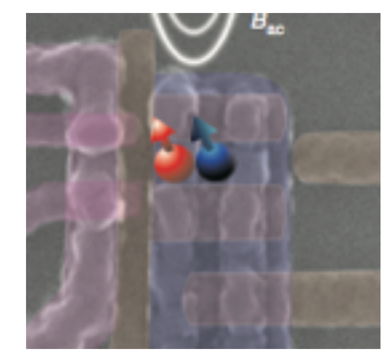
Quantum dots can be reliably coupled!

1-qubit GaAs gates

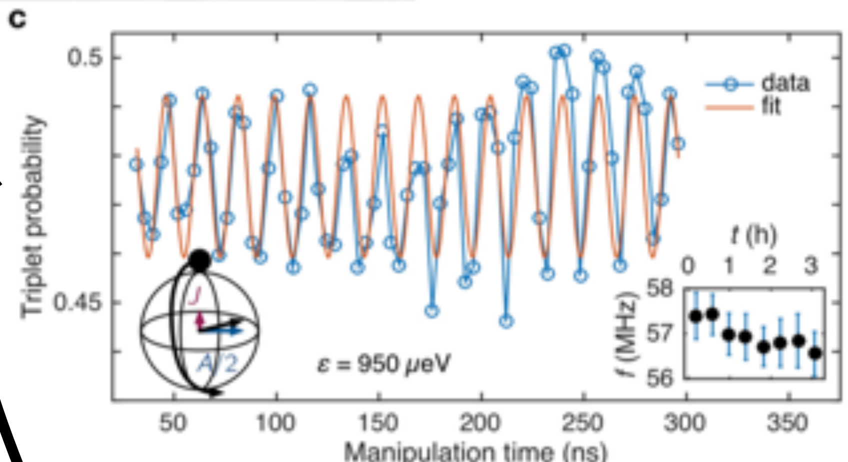


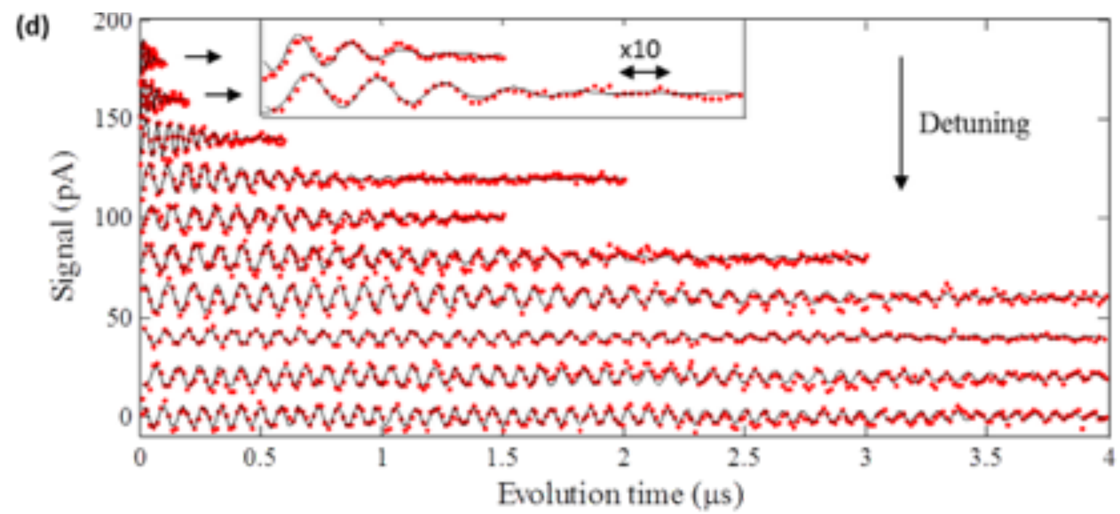
J. Petta, *et al.* Science (2010)

2-qubit silicon gate

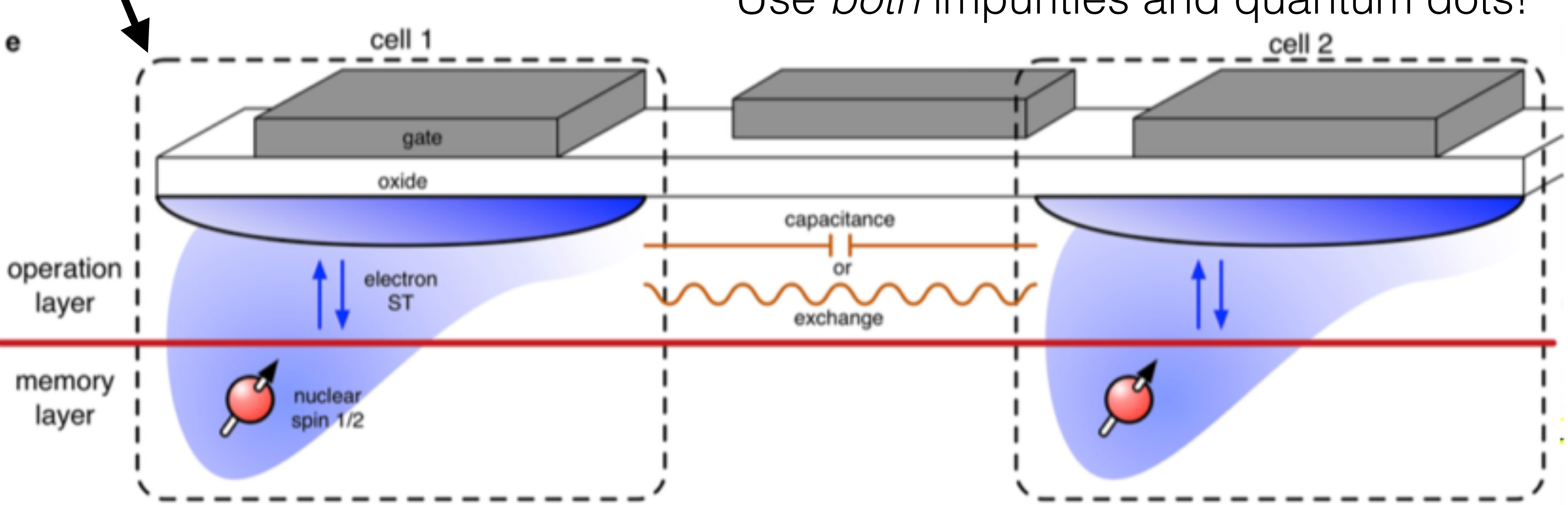


M. Veldhorst, *et al.* Nature (2015).





Use *both* impurities and quantum dots!



P. Harvey-Collard, *et al.*, arXiv:1512.01606.

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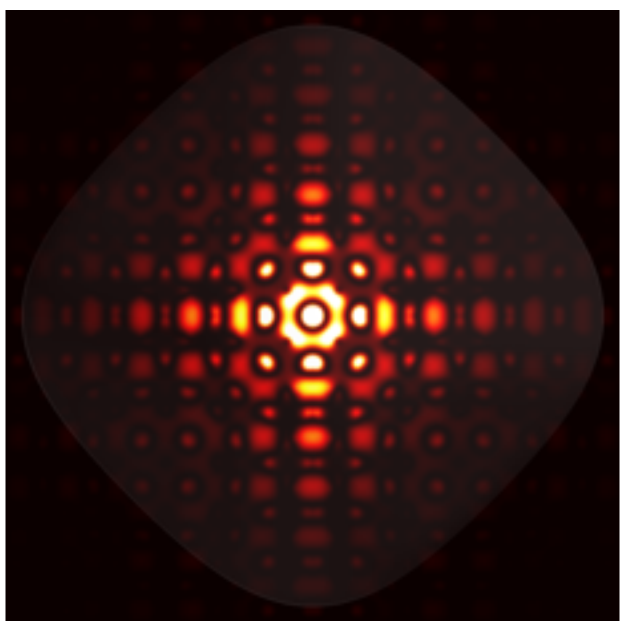

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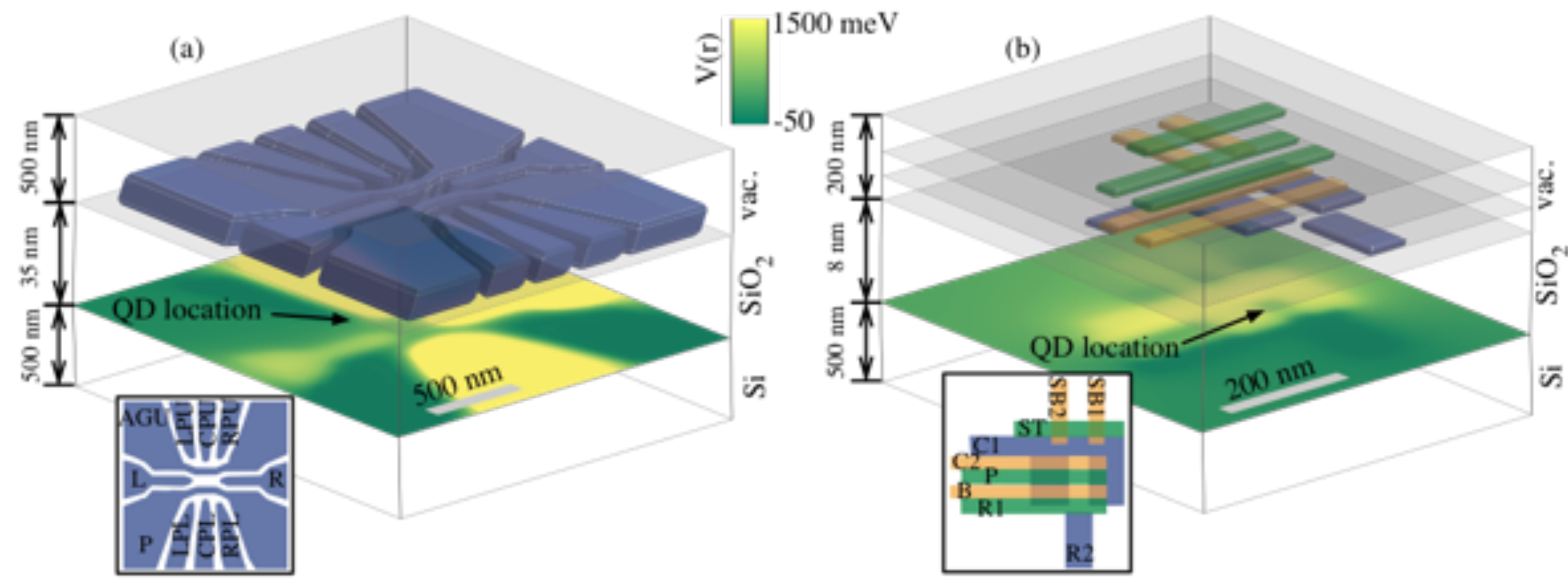
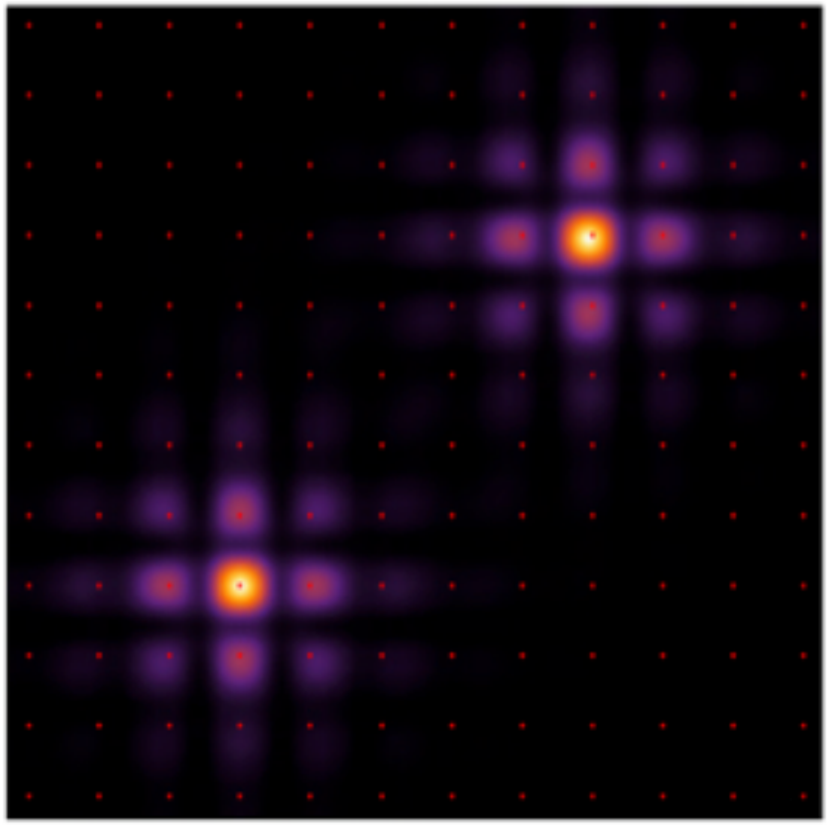


[Gamble, *et al.*, APL (2016)]

Computing the electronic structure of donors in silicon

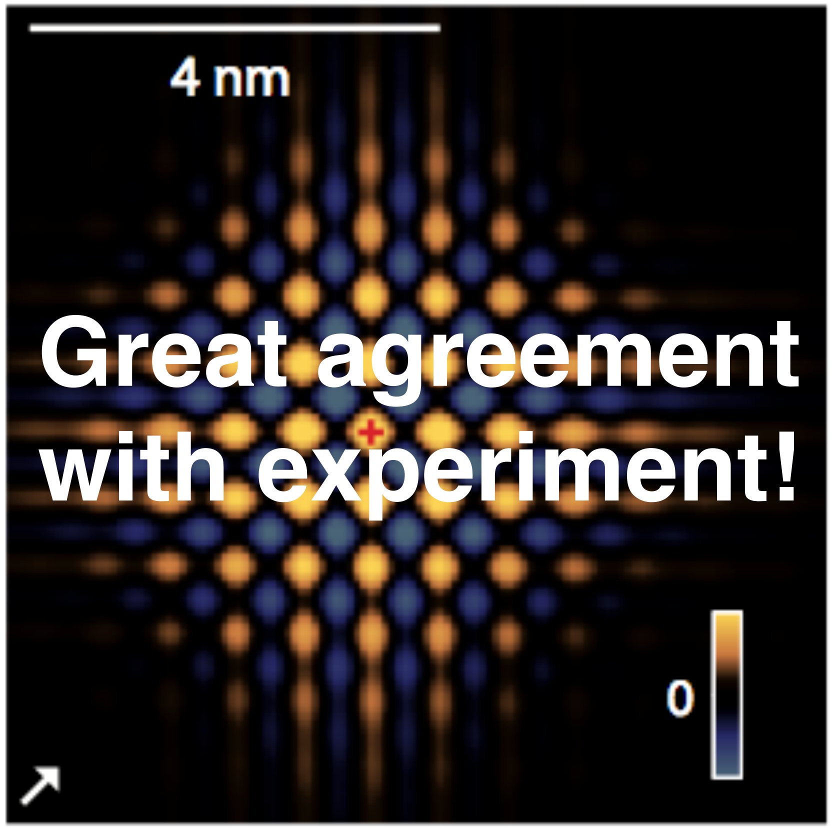
Effective mass



[Pica, *et al*. Phys. Rev. B 89, 235306 (2014)]

Efficient, but only qualitatively reliable. Requires careful application of many approximations.

Atomistic tight-binding



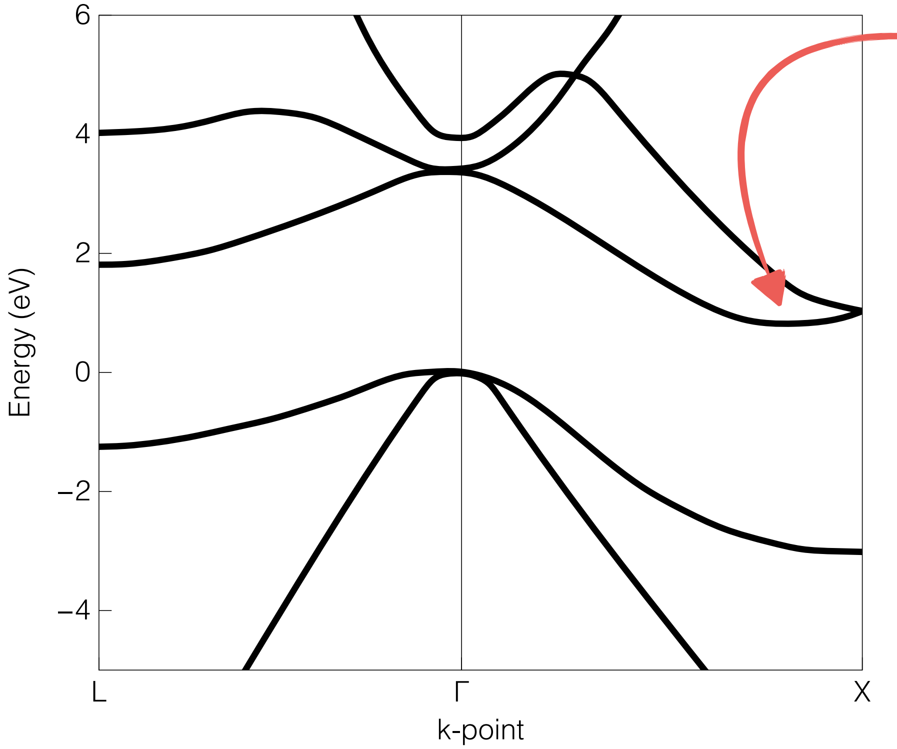
[Salfi, *et al*. Nat. Mat. 13, 605-610 (2014)]

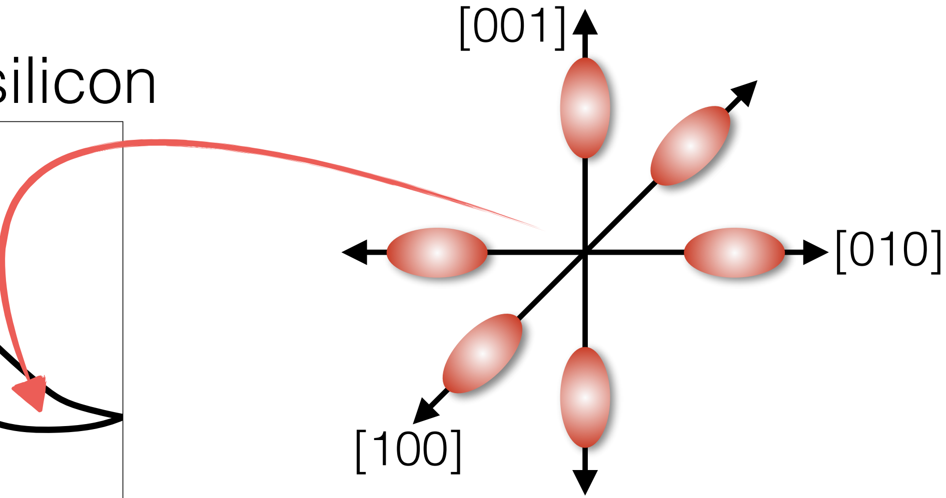
Robust, but computationally intensive.

We want to develop a **quantitatively accurate** effective mass theory - use tight-binding to check for consistency.

Electronic structure of donors in Si

band structure of bulk silicon





conduction band minimum

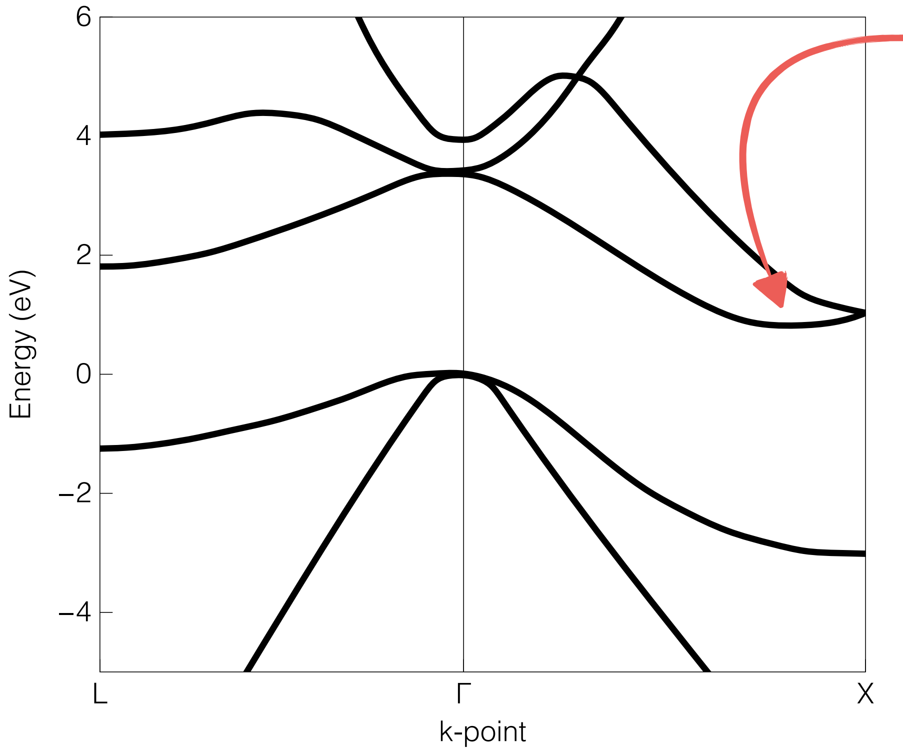
A quantum 'princess and the pea'

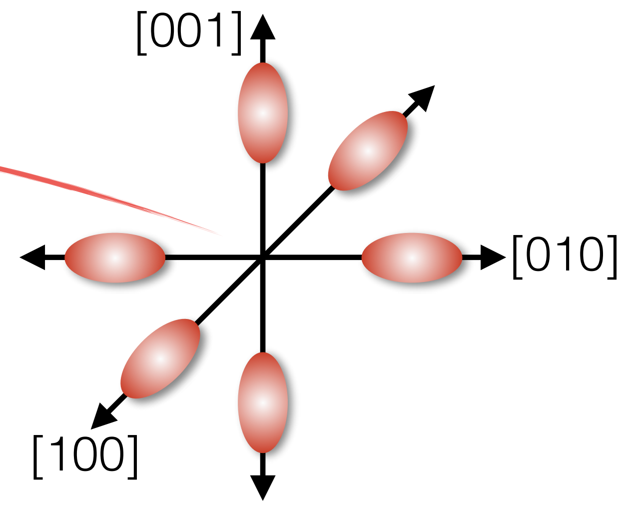
- Long-wavelength (10^{-6} m) electrostatics significantly impacted by small, atomistic features (10^{-10} m)
- Full atomistic modeling of the entire device not feasible: too big
- We designed a multiscale model that can incorporate both atomistic disorder and micron-scale devices.

Illustration by Edmund Dulac, 1911.

Electronic structure of donors in Si

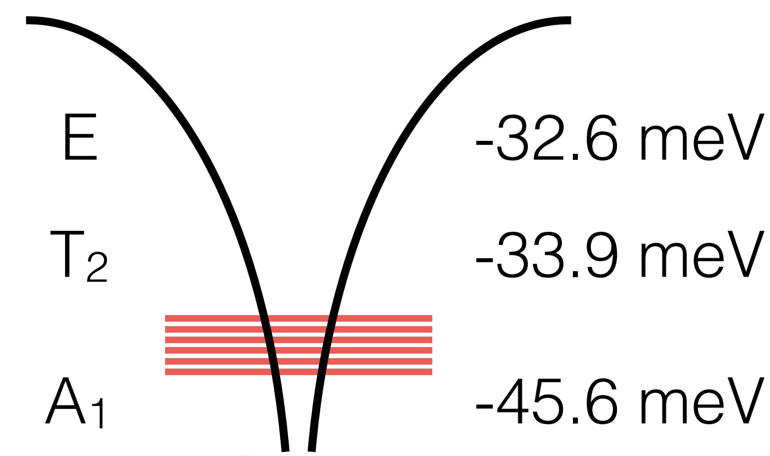
band structure of bulk silicon





conduction band minimum

phosphorous donor



$$\psi(\mathbf{r}) = \sum_j F_j(r) e^{i\mathbf{k}_0^j\cdot\mathbf{r}} u_{\mathbf{k}_0^j}(\mathbf{r})$$

$$u_{\mathbf{k}_0^j}(\mathbf{r}) = \sum_{\mathbf{G}} A_{j,\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}}$$

$$EF_l(\mathbf{r}) = \left(\hat{T}_l + U(\mathbf{r})\right) F_l(\mathbf{r}) + \sum_j V_{lj}^{VO}(\mathbf{r}) F_j(\mathbf{r})$$

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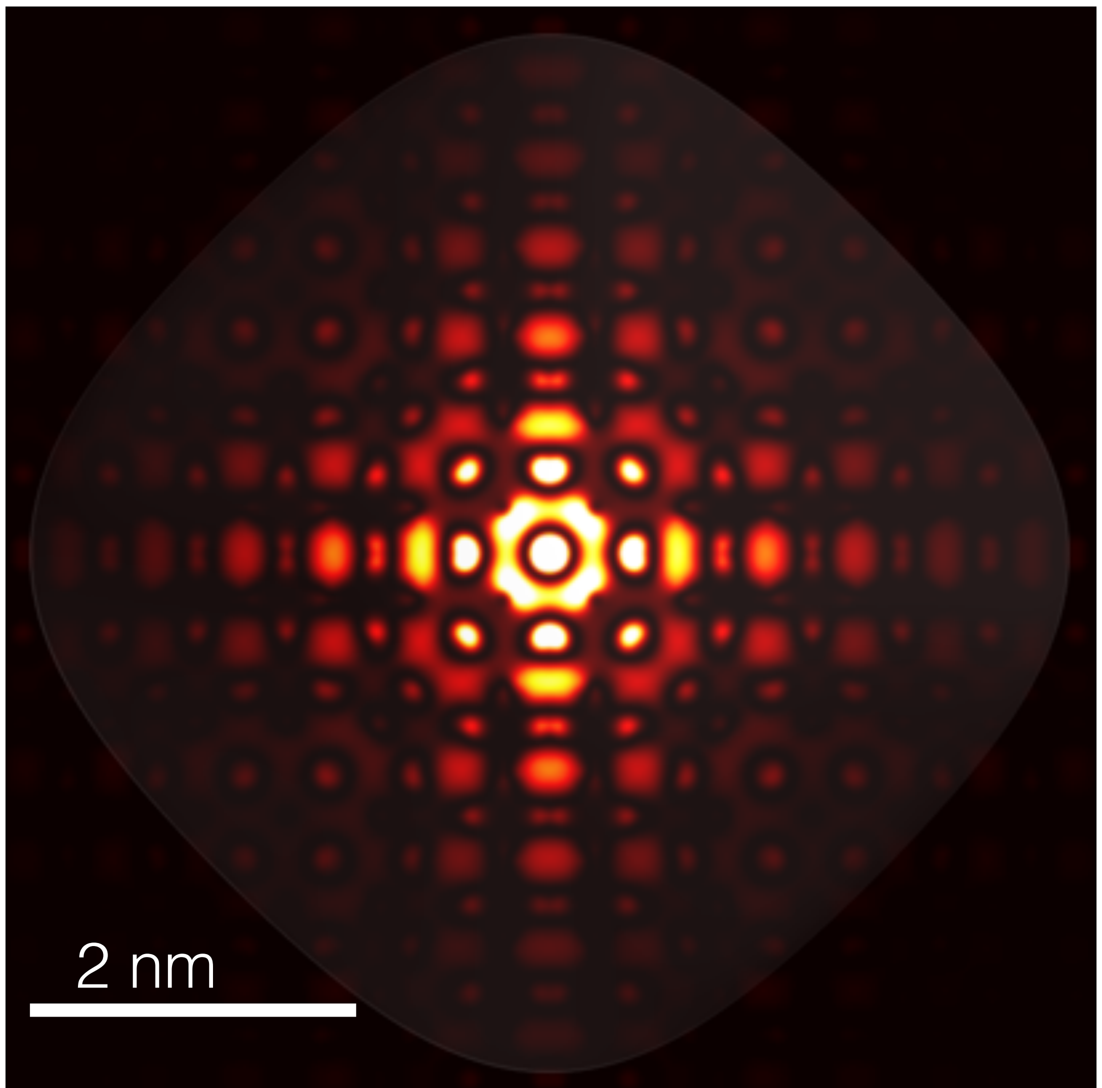
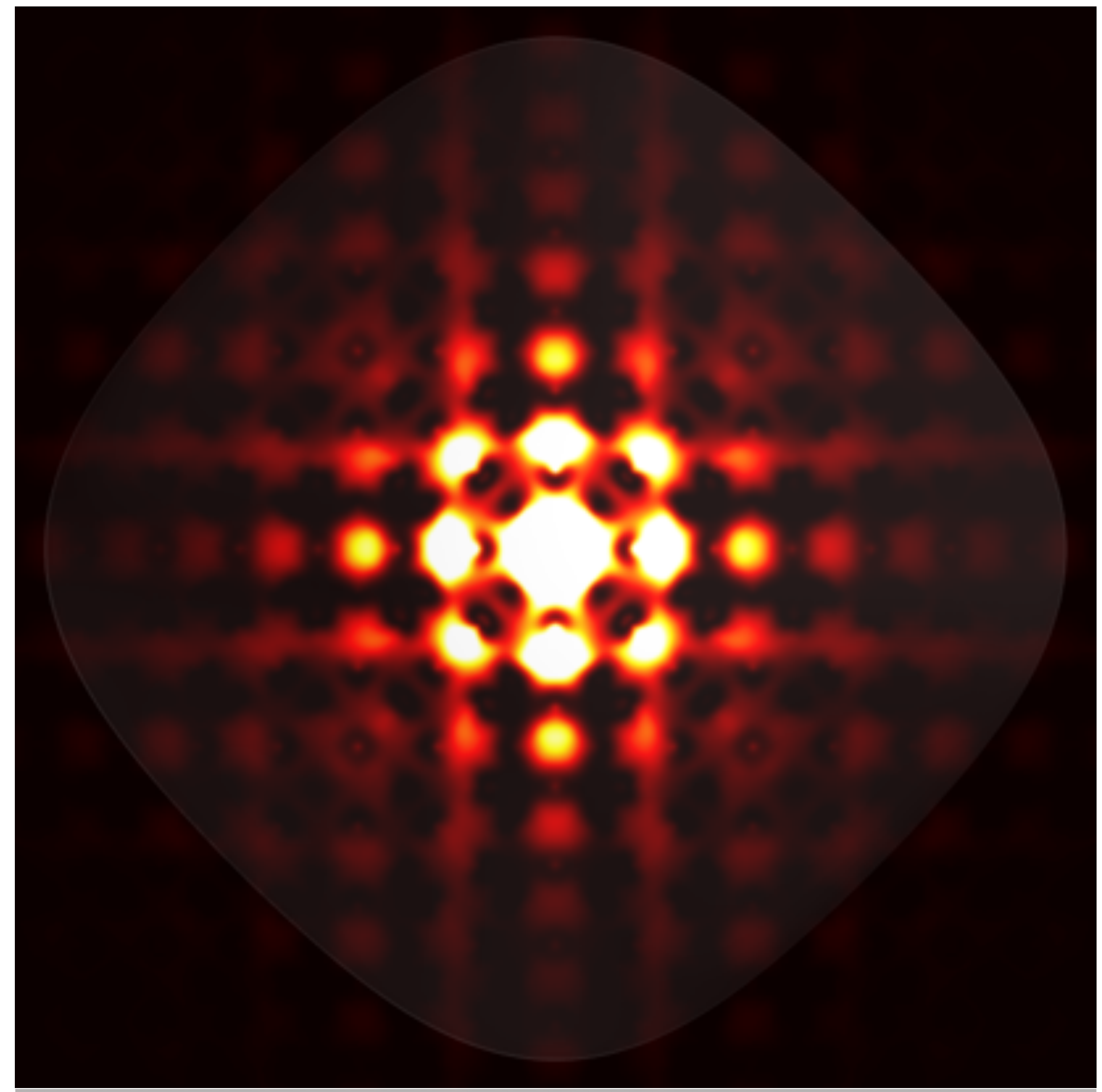
Gamble, *et al.*, PRB (2015).

The donor wave function is sharply peaked and oscillatory

Effective mass calculation



Atomistic calculation (NEMO 3D)



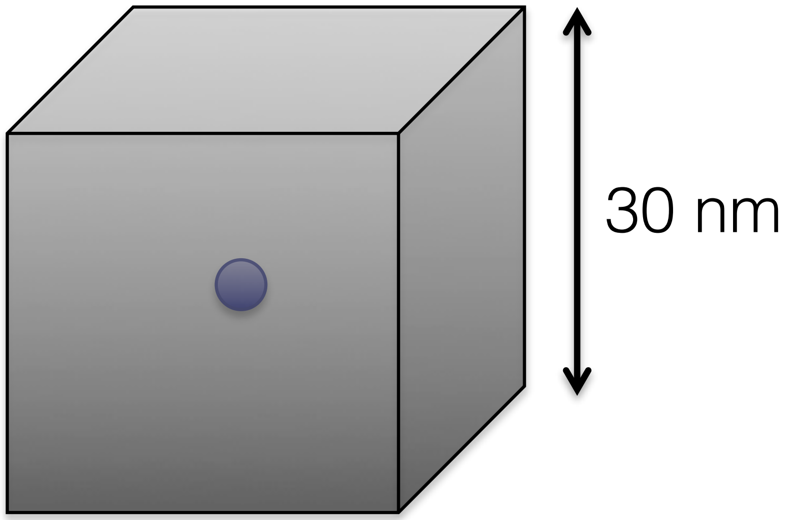
Gamble, *et al.*, PRB (2015).

Use effective mass to probe tunnel coupling: a critical figure of merit

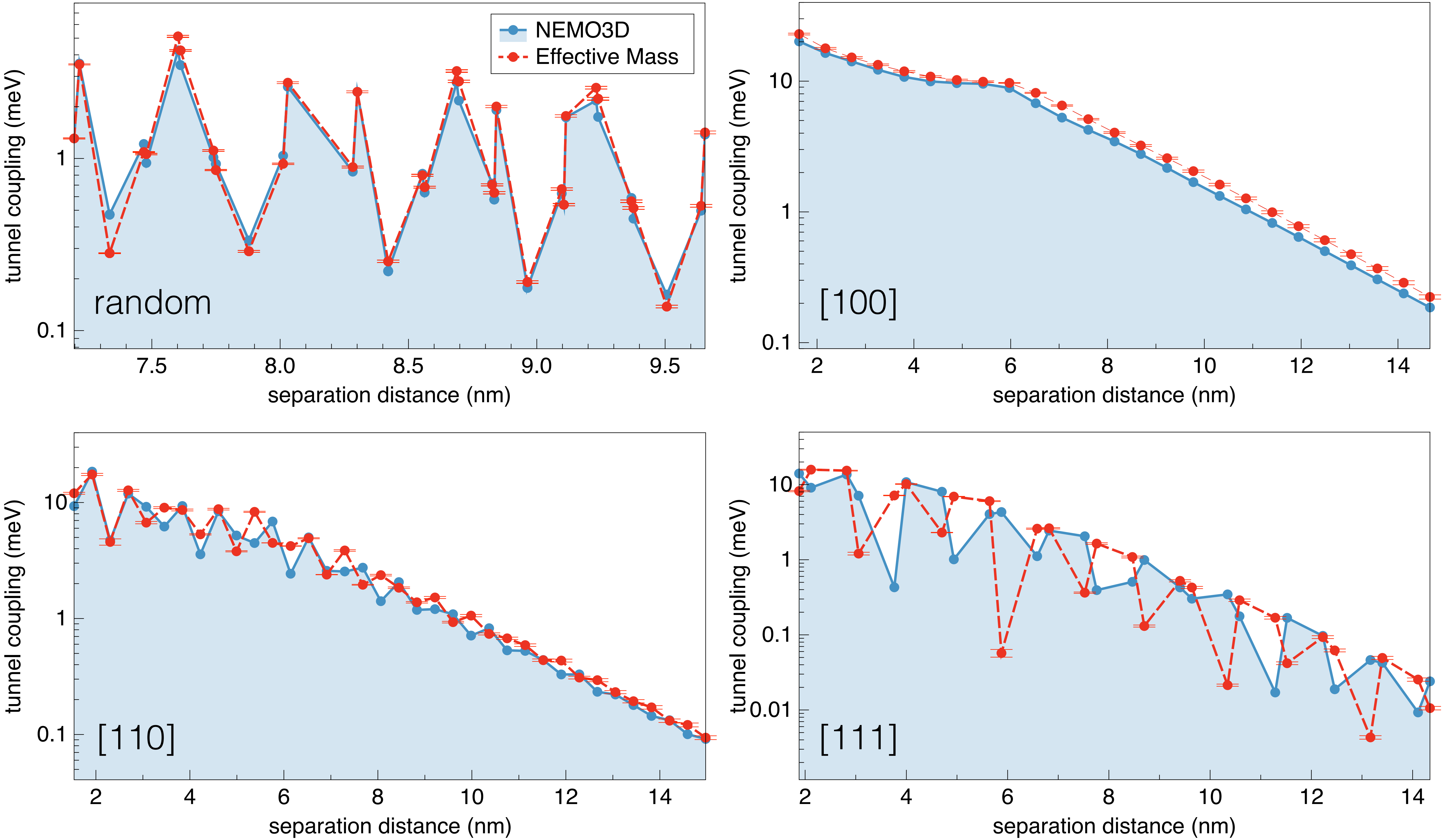
- **Tunnel coupling** is the difference between the lowest two eigenstates of a two-donor problem:

$$t = E_1 - E_0$$

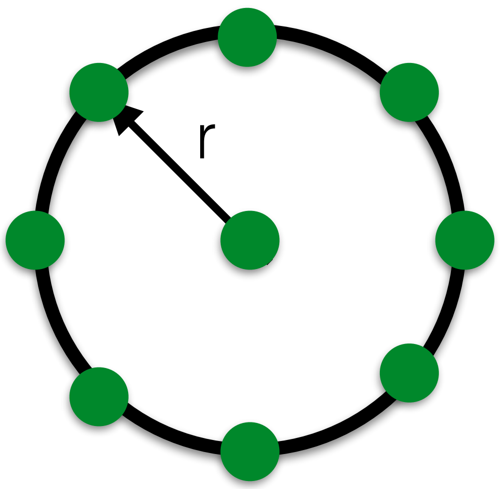
- Tells us about the coupling strength: important for electron-electron interactions and electron transport.
- We compute the tunnel coupling between one donor at the origin and the second at **all possible locations** in a 30 nm cube (~1.3 million locations).
- Effective mass code took about **1.5 hours per shot on one core** = ~ 150k compute-hours total (after using symmetry).

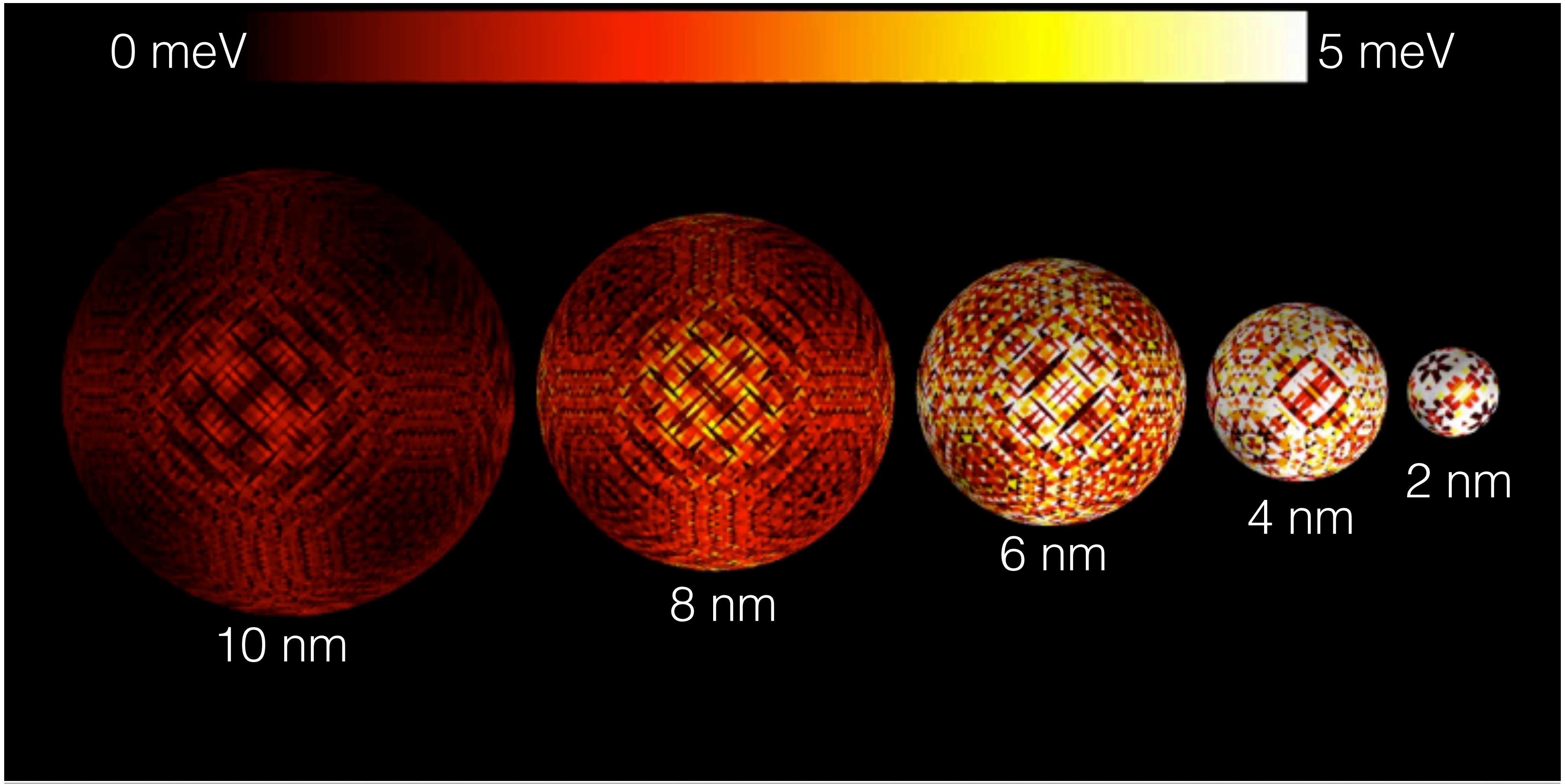


Effective mass and tight-binding agree: tunnel coupling is very sensitive to position



Probing the entire range of tunnel couplings, there are no stable regions





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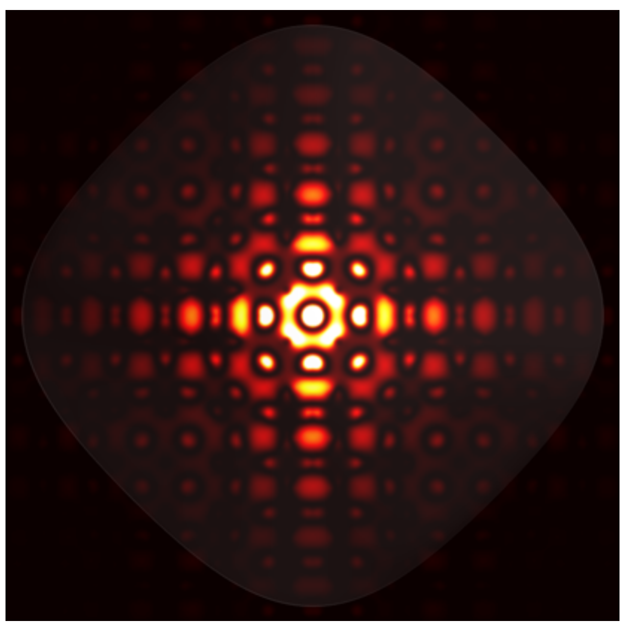

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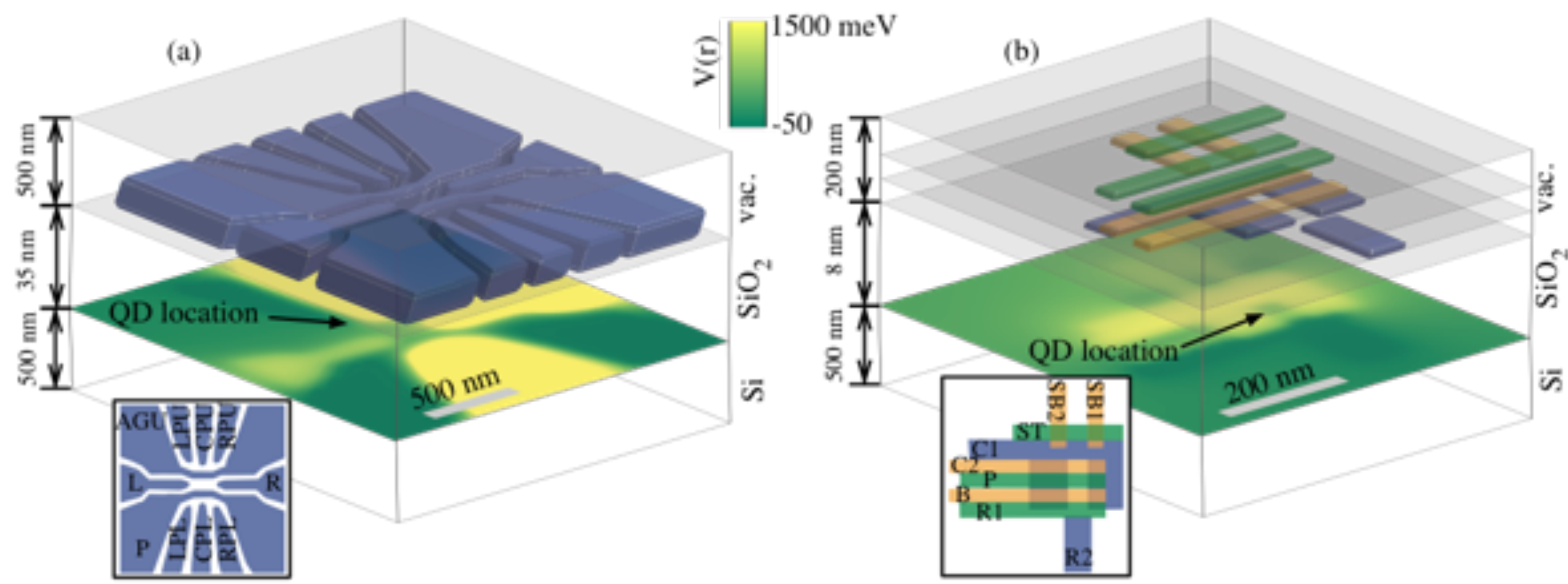

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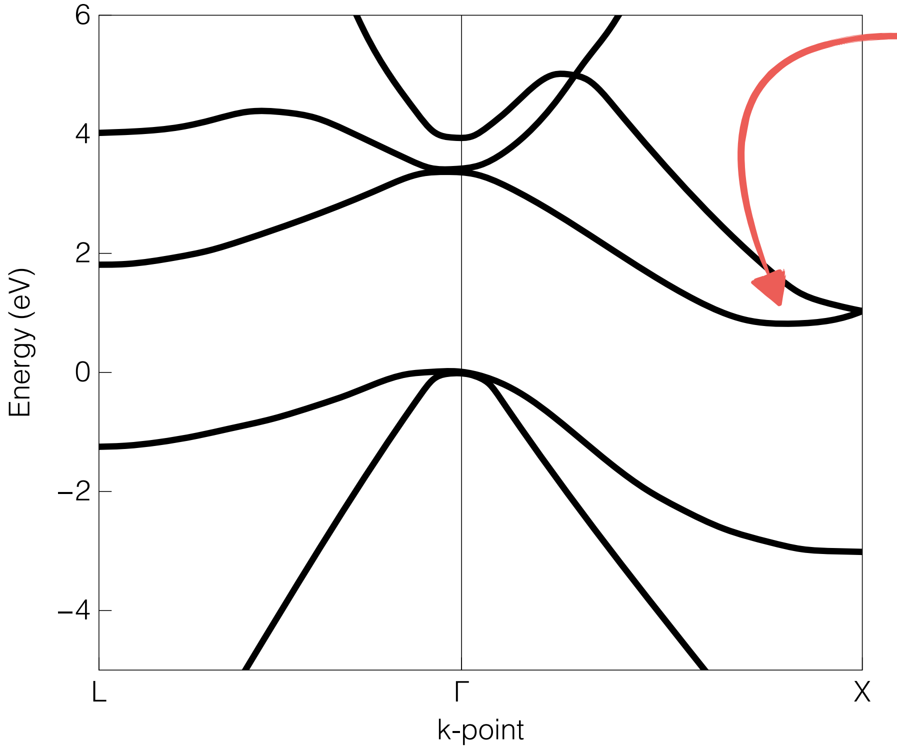
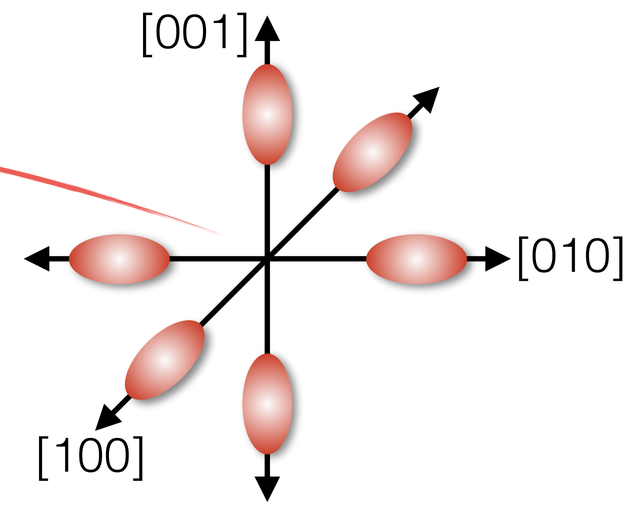
Electronic structure of quantum dot electrons in Si

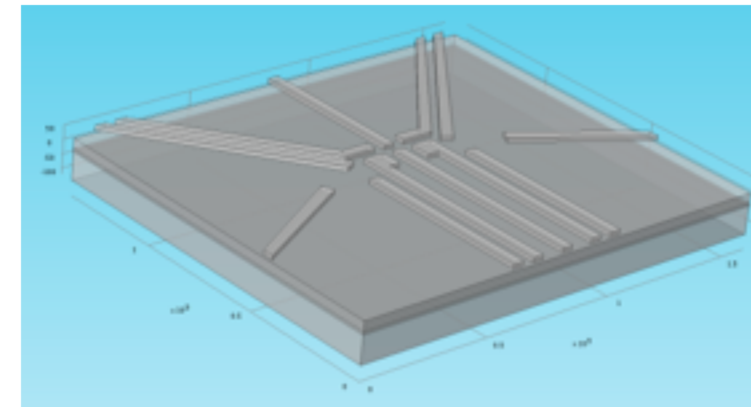
band structure of bulk silicon



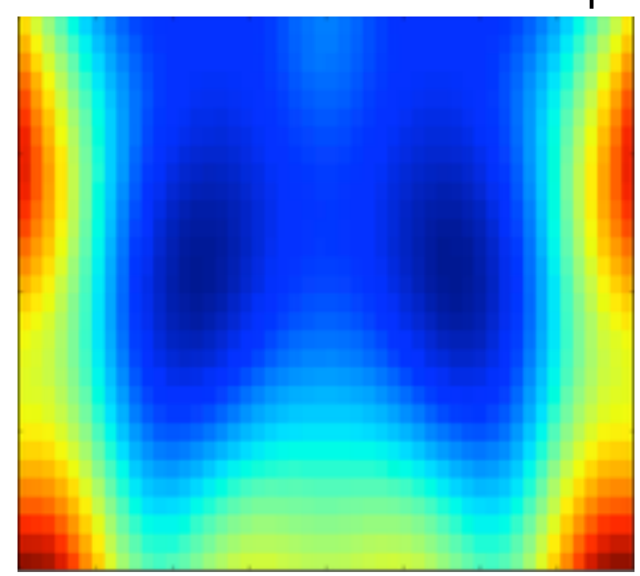


conduction band minimum

Finite element model



electrostatic landscape



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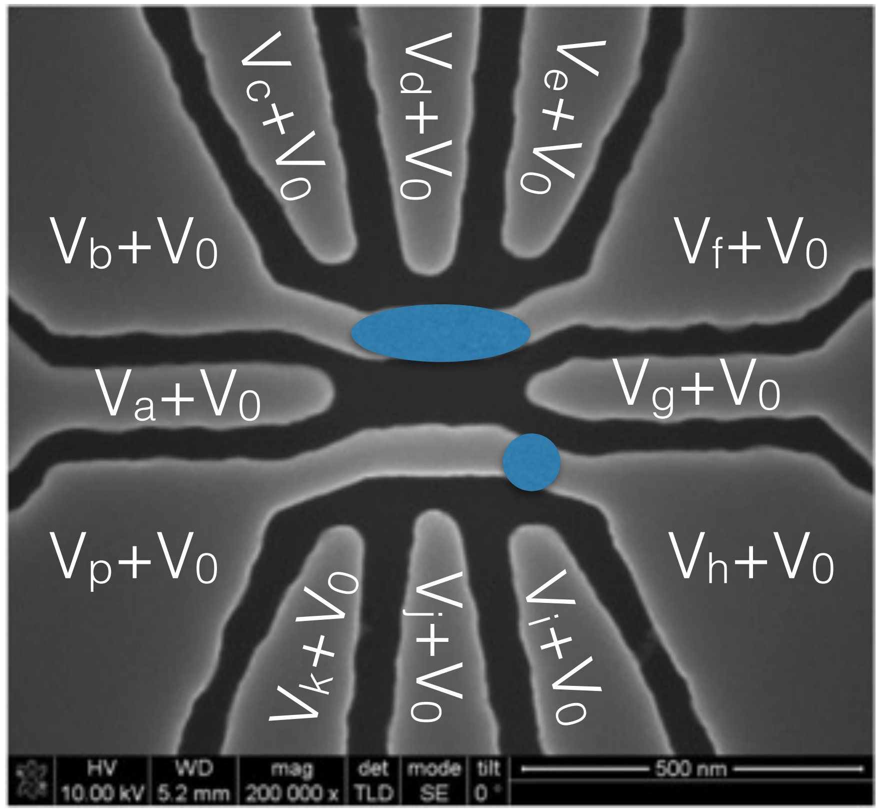
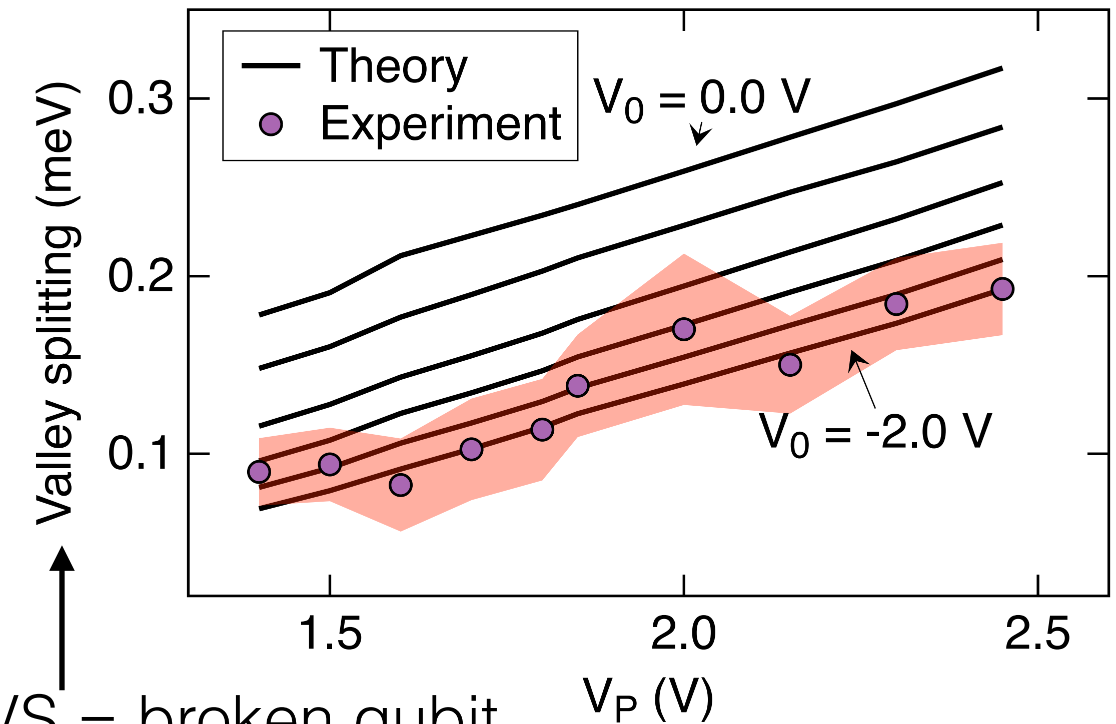
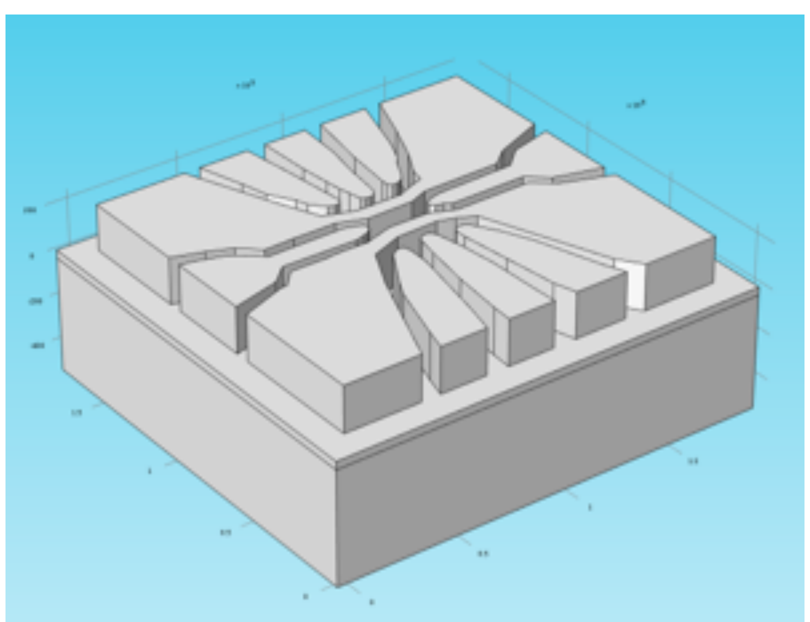
Gamble, *et al.*, APL (2016).

Case study: valley splitting directly from a device design and experimental voltages.

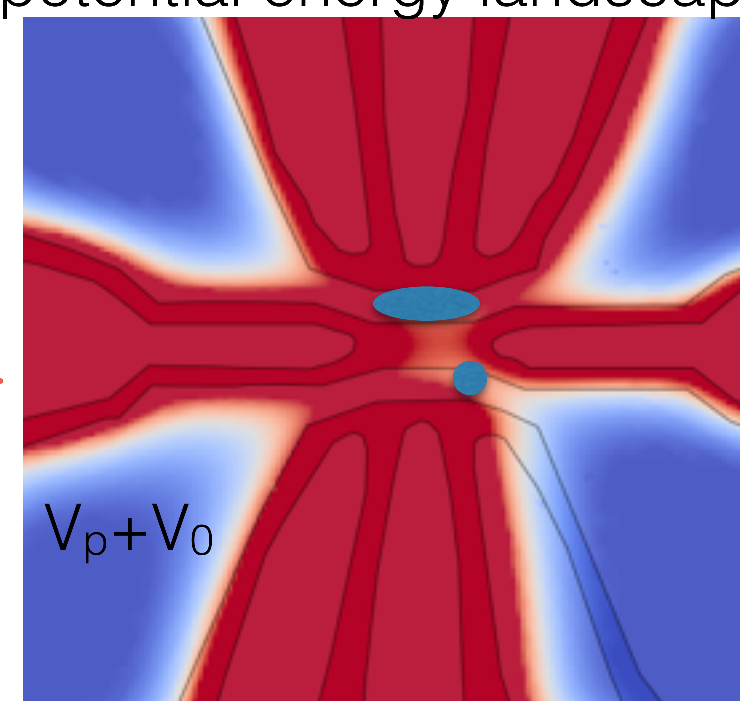




small VS = broken qubit



potential energy landscape



To confirm the results, we modeled a second system.

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ARTICLE

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Spin-valley lifetimes in a silicon quantum dot with tunable valley splitting

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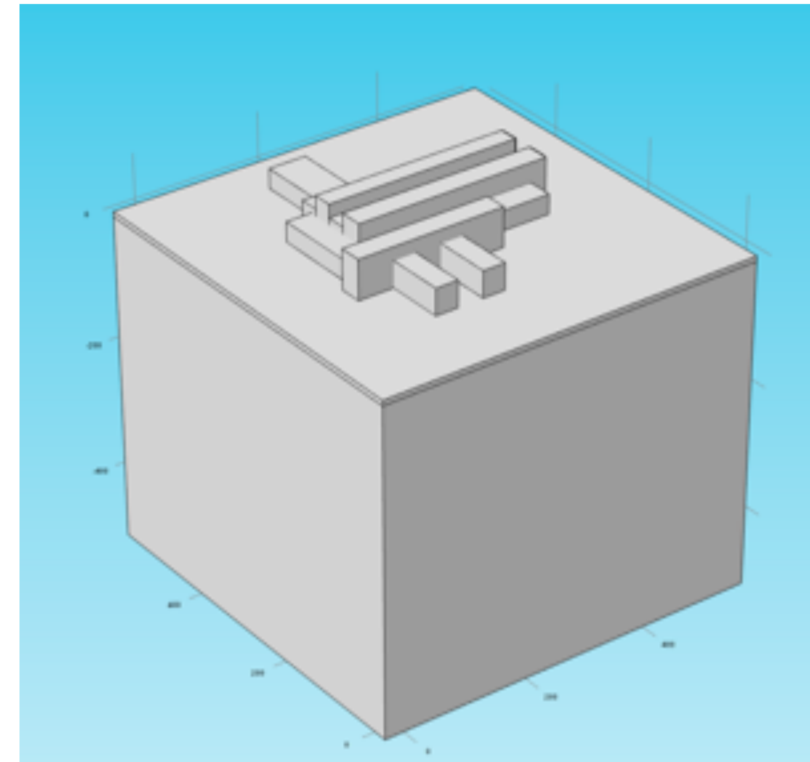
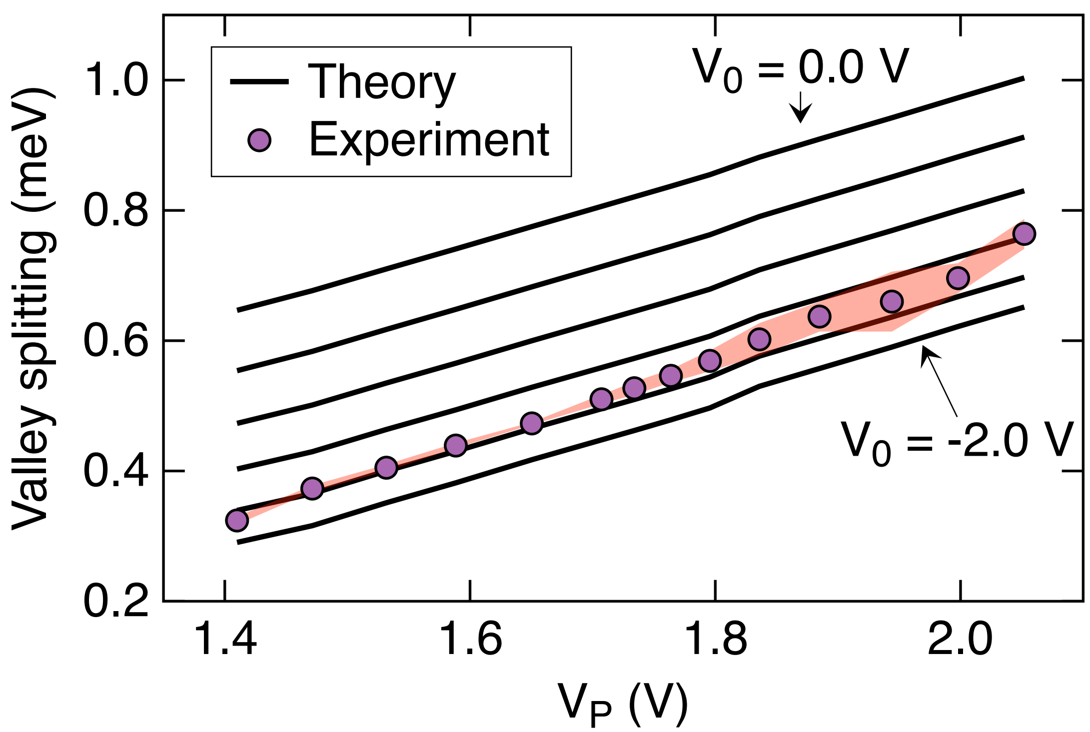
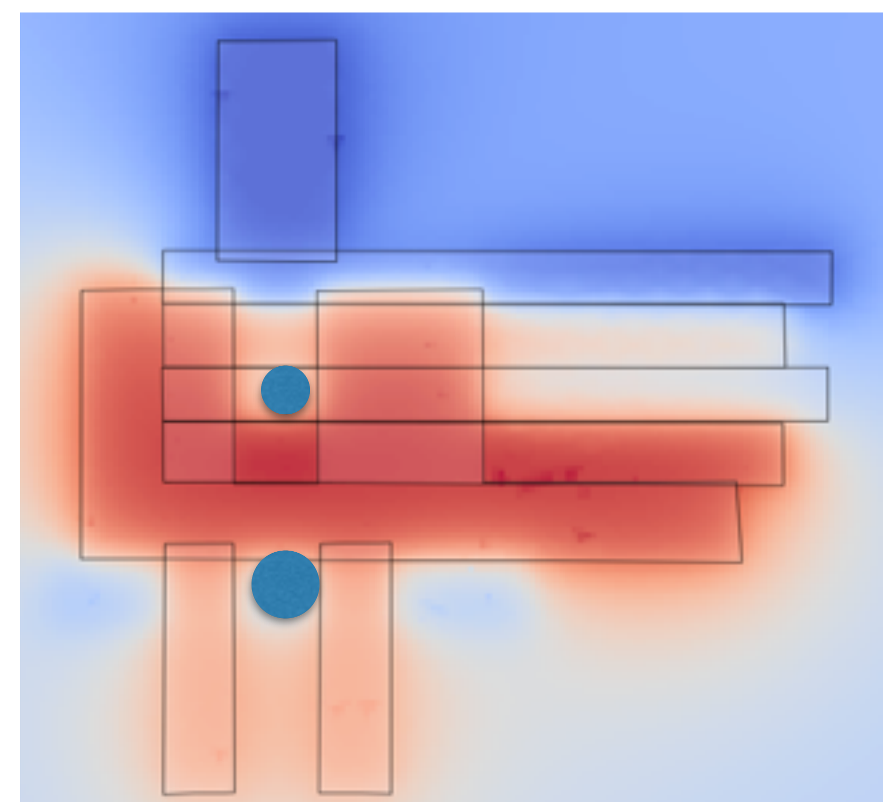
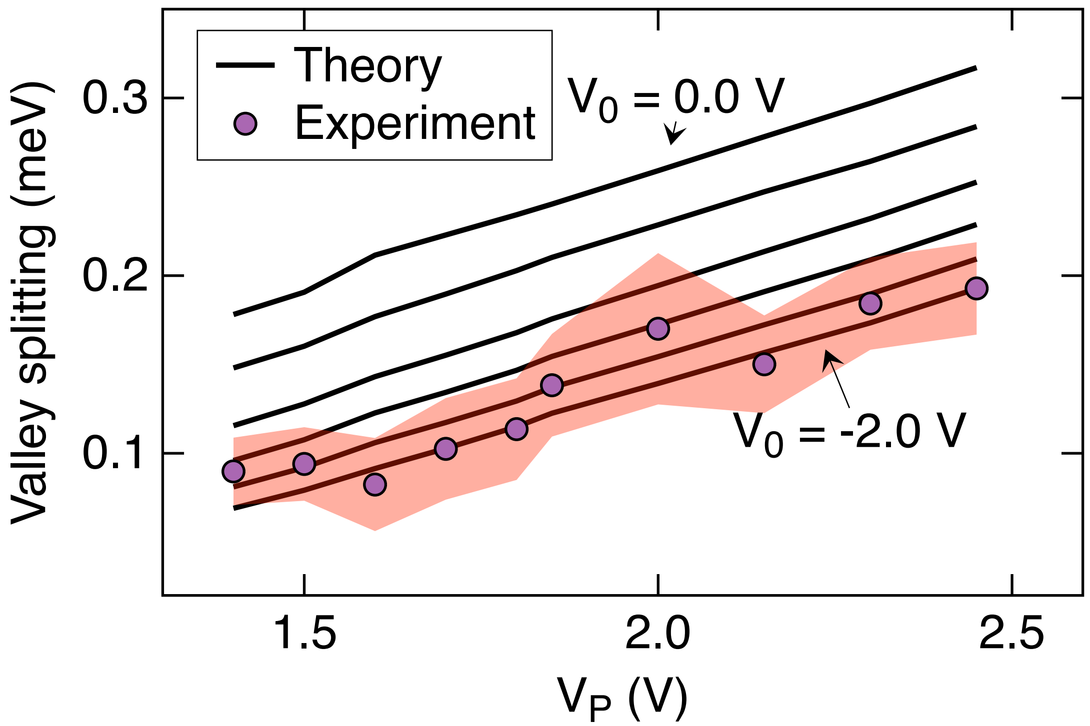
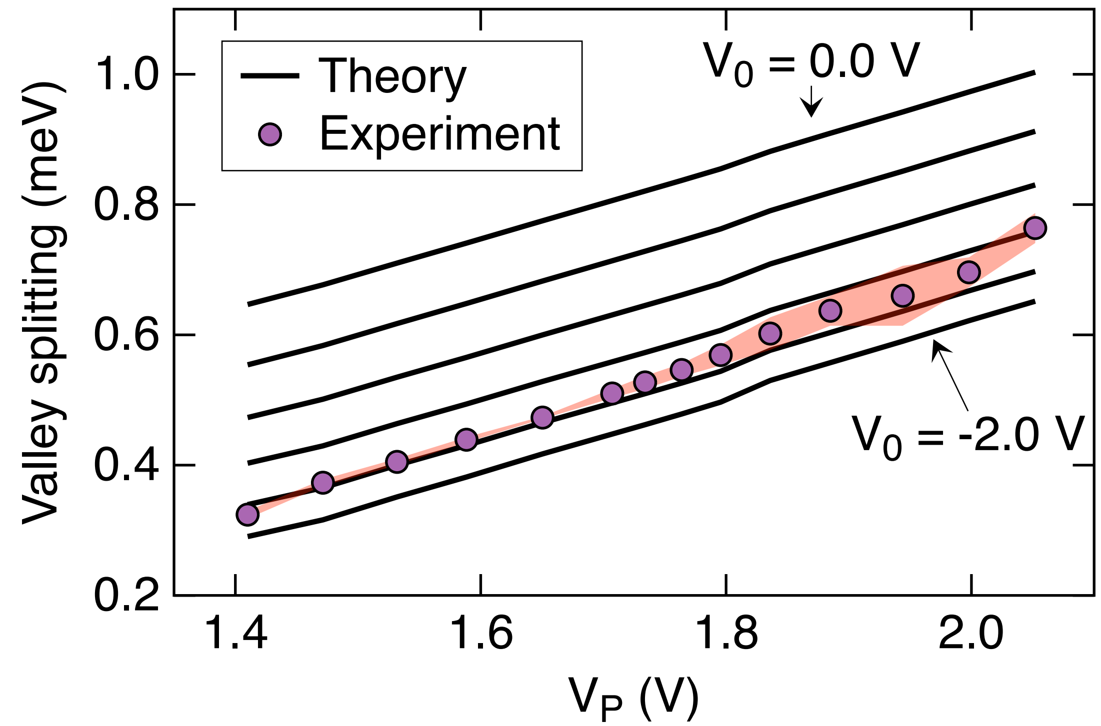






In both cases, the theoretical predictions are consistent with experiment





- Very different fabrication processes and device geometries.
- Since small VS leads to broken qubits, we need to be able to accurately model it to design qubit structures.
- The theoretical predictions are consistent between devices, despite many differences in fabrication (and large spacetime separation).
- In practice, threshold voltages tend to be smaller magnitude than 1.8 V - this discrepancy is consistent with detailed statistical disorder study.

Gamble, *et al.*, APL (2016).

Combining both species of artificial atoms

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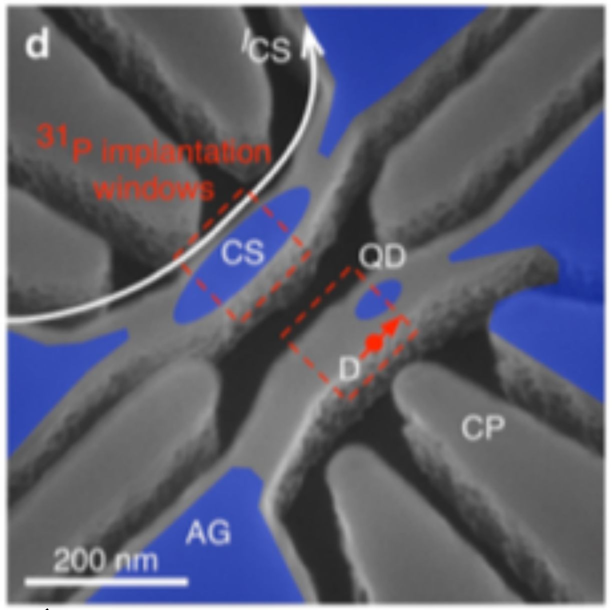
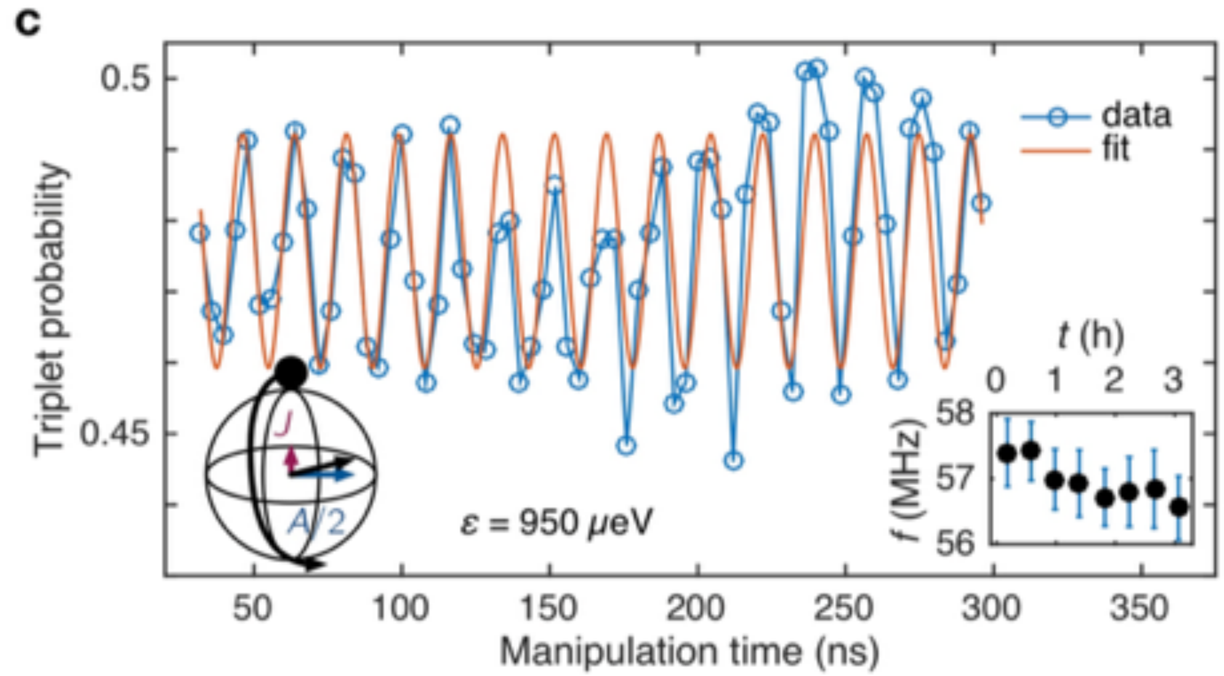
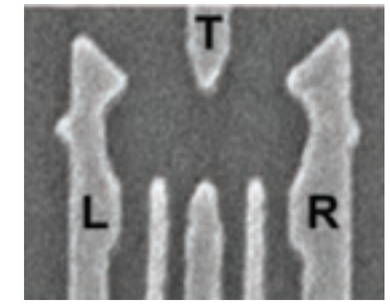




One cell has been demonstrated in experiment.

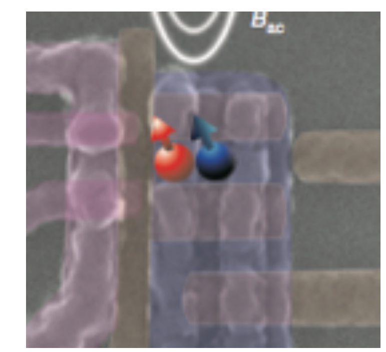
Quantum dots can be reliably coupled!

1-qubit GaAs gates



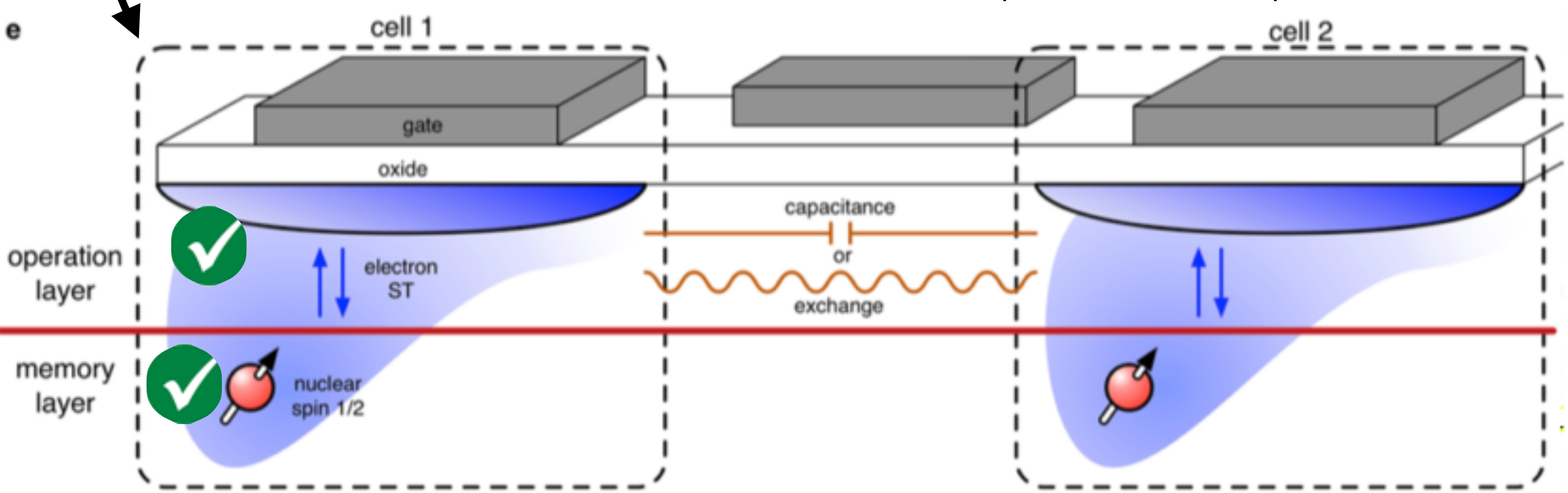
J. Petta, *et al.* Science (2010)

2-qubit silicon gate



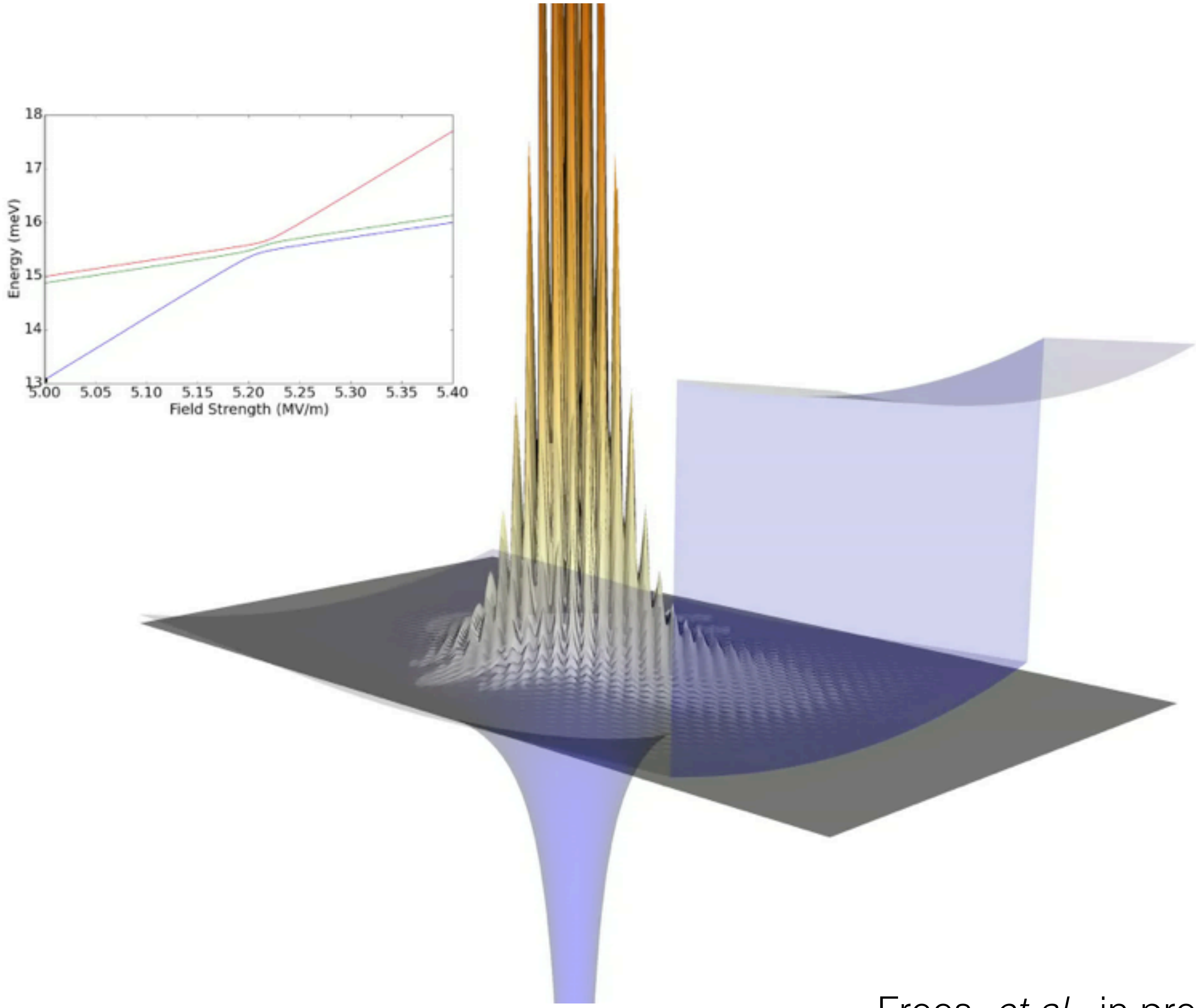
M. Veldhorst, *et al.* Nature (2015).

Use *both* impurities and quantum dots!



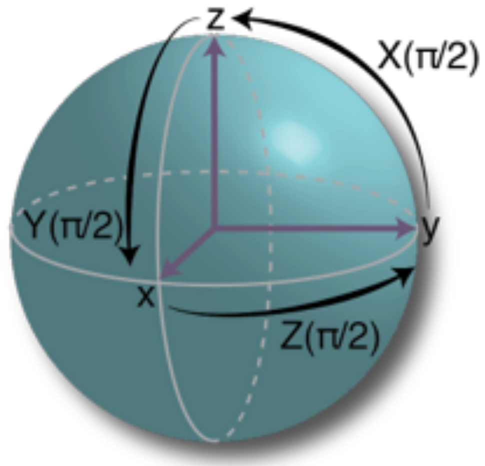
P. Harvey-Collard, *et al.*, arXiv:1512.01606.

Putting the pieces together: impurity + interface dot

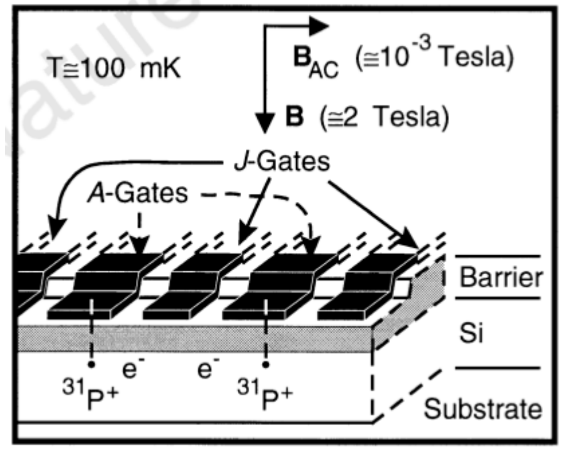


Frees, *et al.*, in preparation.

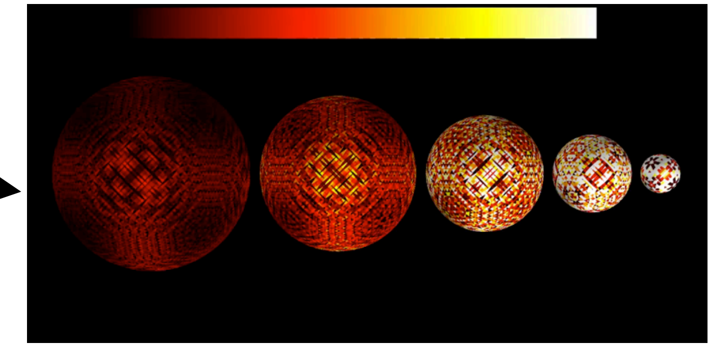
Summary



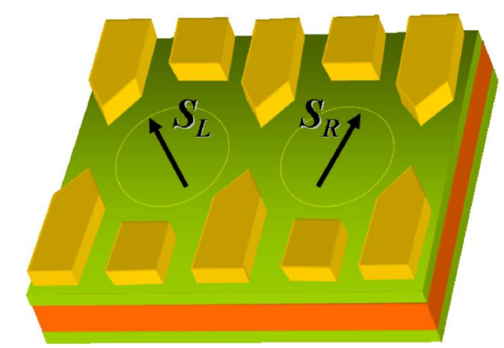
Want to encode qubits in a convenient physical system.



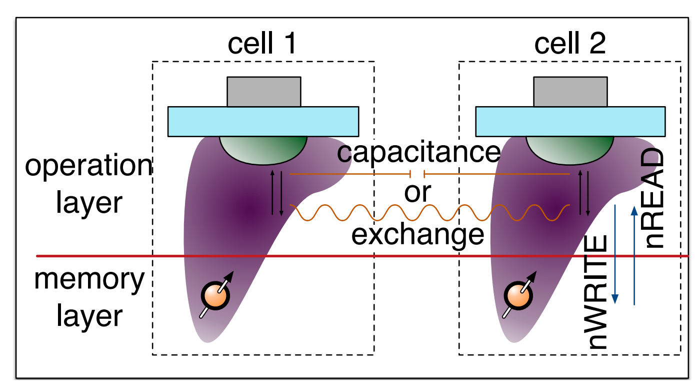
Donors in silicon seem ideal…



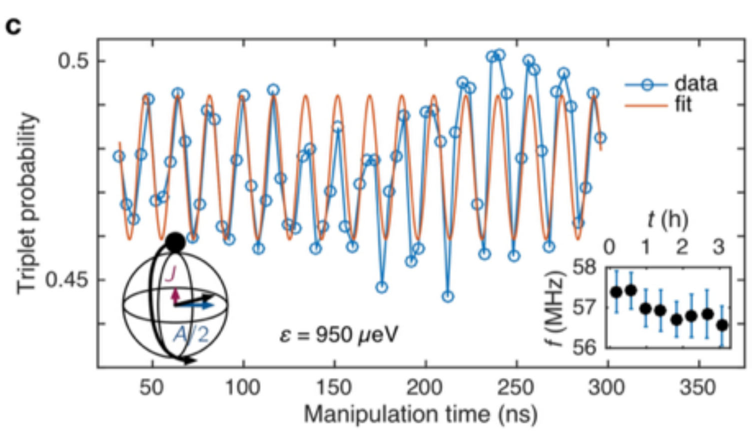
…but they can't be reliably coupled!

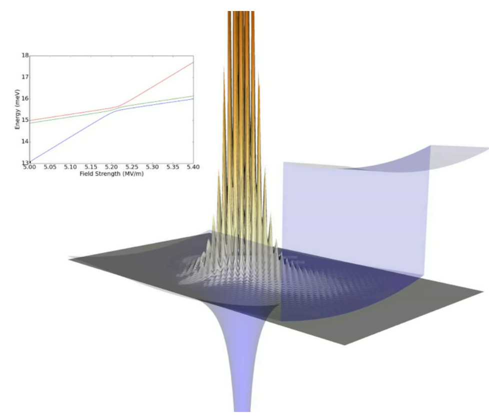


Quantum dots can be coupled more easily.



Mediate donor-donor interactions through dots.





Experimental evidence + unified multiscale device model.

Thanks!

SNL Theory collaborators

- Andrew D. Baczewski
- N. Tobias Jacobson
- Inès Montaño
- Jonathan E. Moussa
- Richard P. Muller
- Erik Nielsen
- Leon Maurer

SNL experiment collaborators

- Malcolm Carroll
- Patrick Harvey-Collard
- Martin Rudolph

External collaborators

- A. S. Dzurak (UNSW)
- Adam Frees (U-Wisconsin)
- A. Rossi (Cambridge)
- C. H. Yang (UNSW)

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Backup Slides

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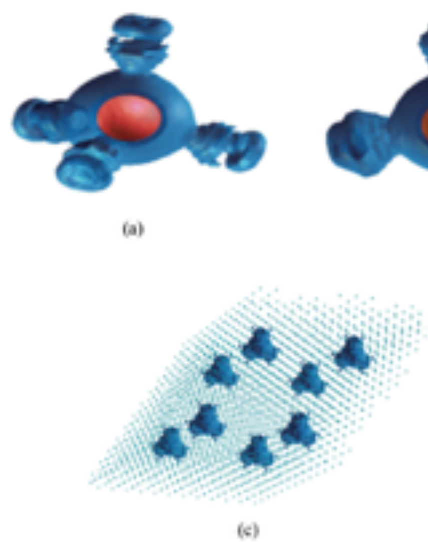
Find a good central cell and donor wave function by two-stage optimization

The bulk-screened coulomb potential is too weak to explain observed binding energies on its own. We need to modify it to get the energies right.

Central cell

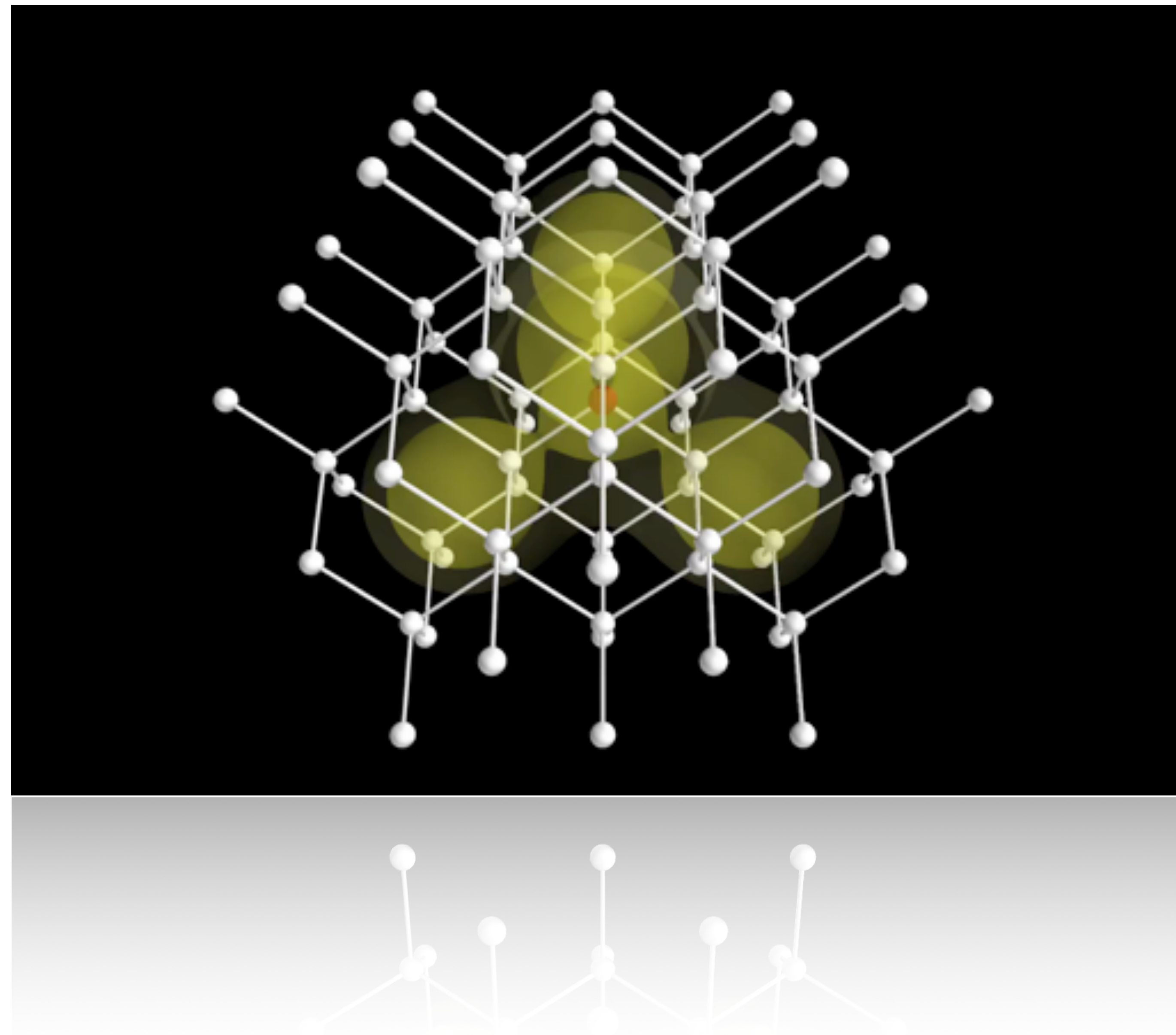
Variational ground state



Greenman *et al.*
PRB **88,** 165102 (2013)

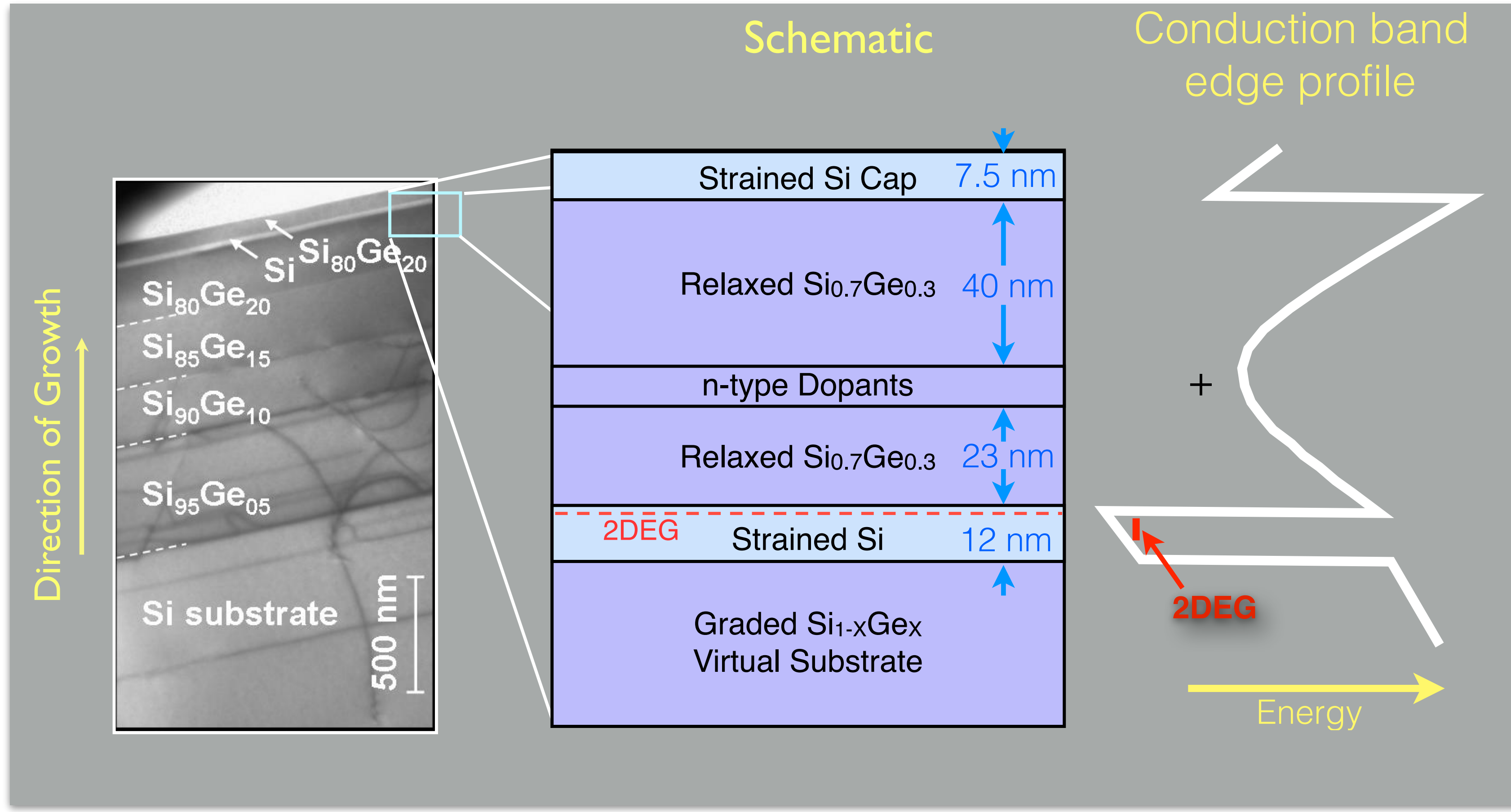
Objective:

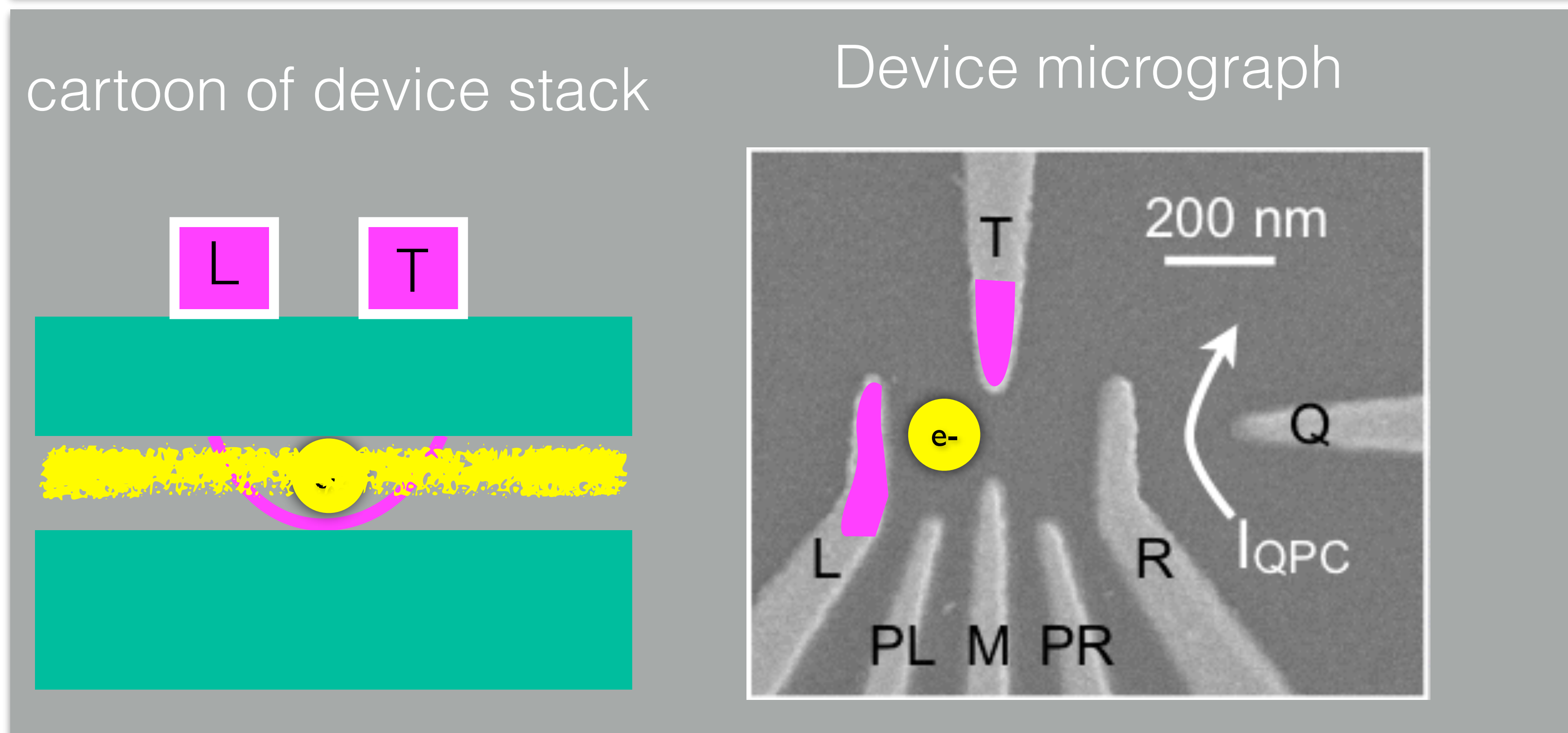
E	-32.6 meV
T_2	-33.9 meV
A_1	-45.6 meV



Quantum dot electron spin qubits

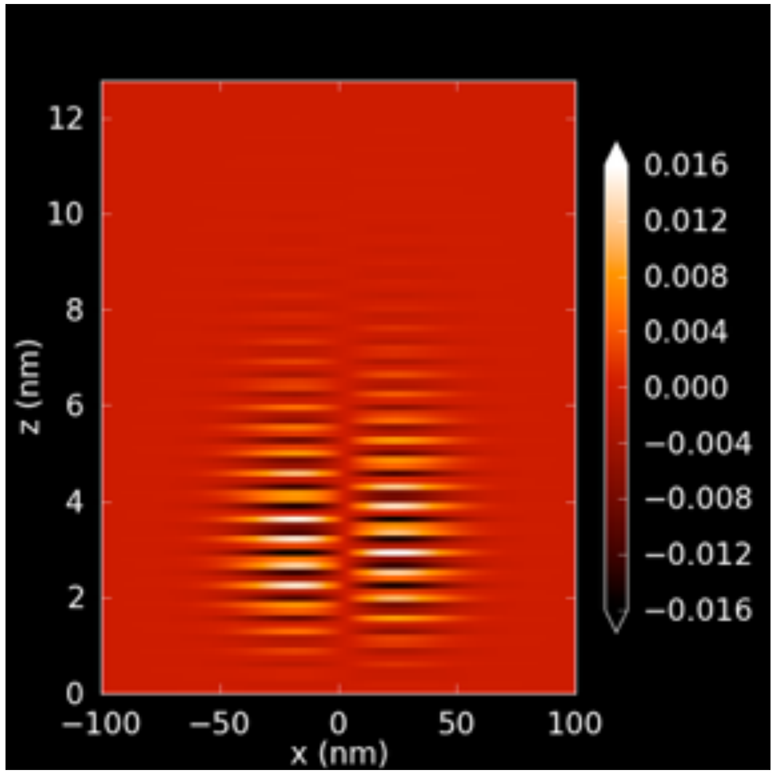
- One example is electrostatically defined, Si/SiGe quantum dots
- Electrons trapped below surface in a two-dimensional electron gas (2DEG) formed in a quantum well of a semiconductor heterostructure
- Once confined in the well, further confined to a quantum dot with electrostatic depletion gates patterned on the top of the sample
- Electron number is controlled by electrically tuning the depletion gates



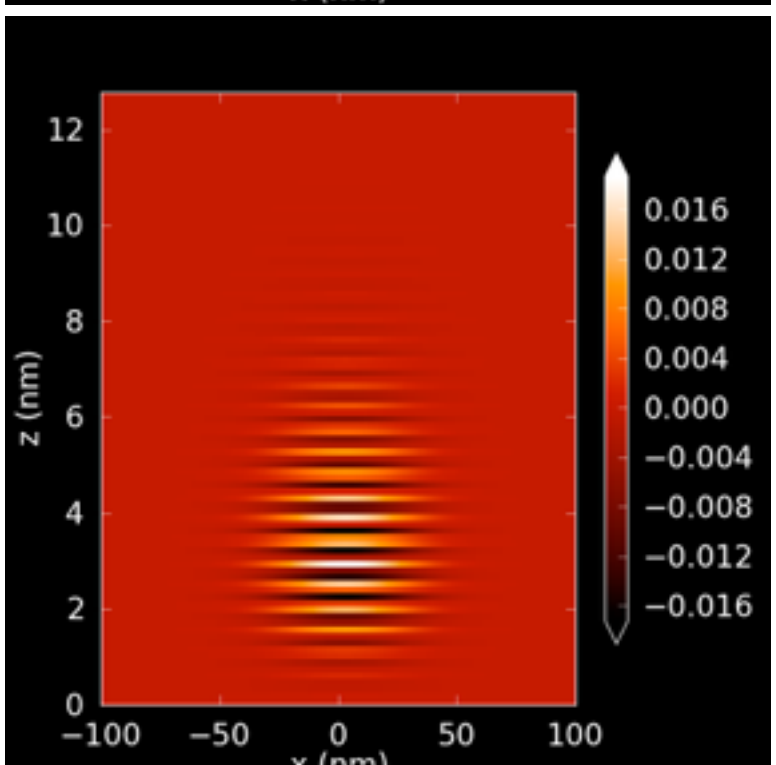


As with donors, the “valley physics” of dots is complicated and multiscale

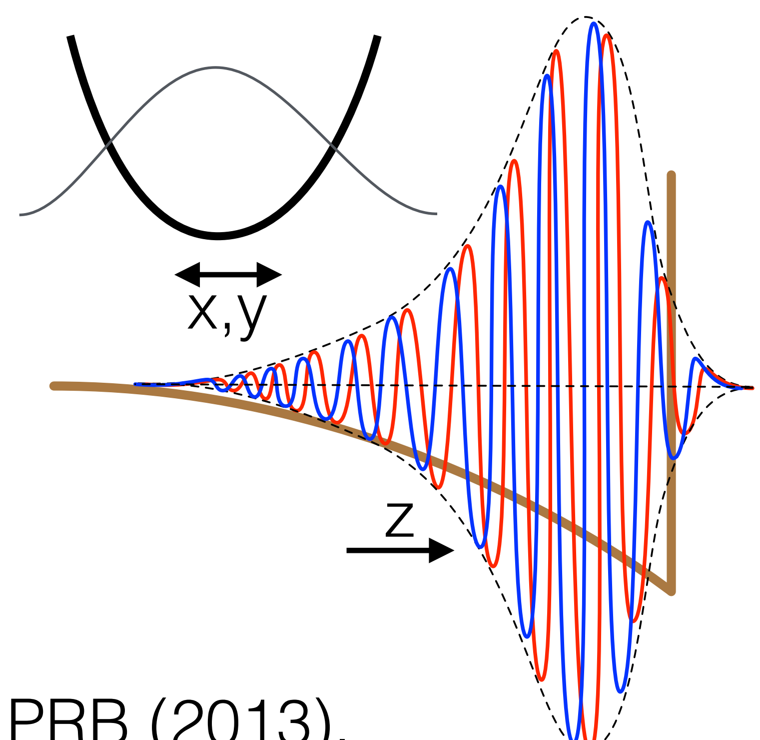
1st excited state



ground state



- Complicated interference patterns develop between different conduction band valleys.
- In real space, the electronic wave function exhibits fast oscillations along the direction of the semiconductor stack (z), modulated by a slow envelope.
- Since we want a two level system, we can’t have extra degrees of freedom laying around!

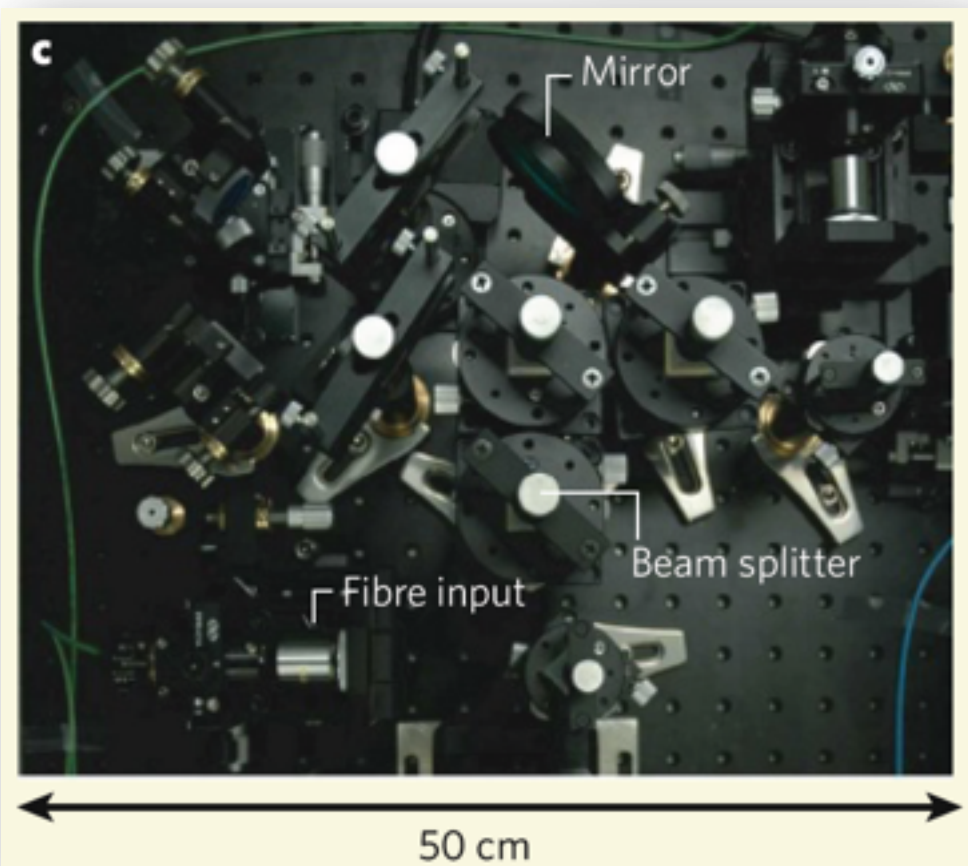


Gamble, *et al.* PRB (2013).

What does this actually look like in a lab?

PMT

APD



Optical Table

Dilution

Refrigerator

Low T Superconducting

Apparatus

Semiconductor qubits live in here
close to absolute zero

Currently, many different techniques see use in modeling semiconductor QIP systems.

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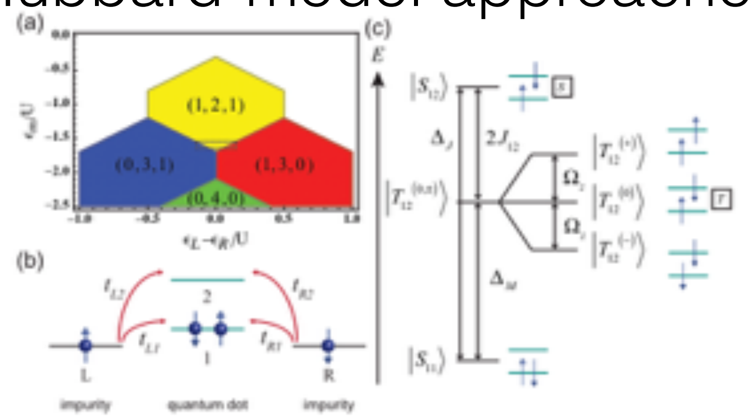
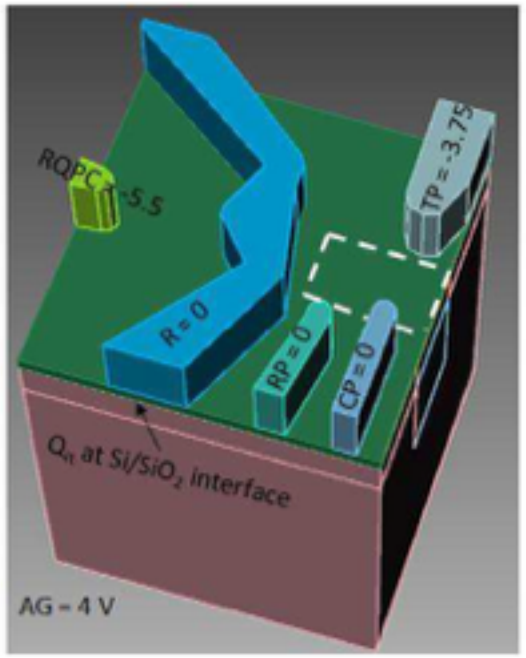
Hubbard-model approaches



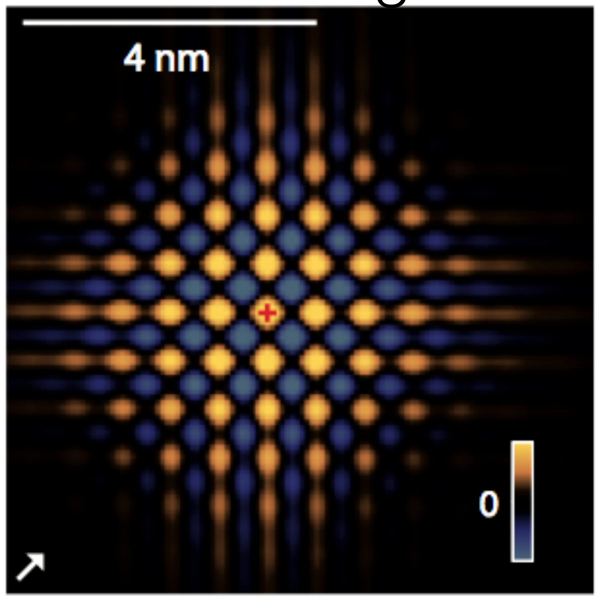
[Srinivasa, et al. arXiv:1312.1711 (2014)]

Device-scale methods



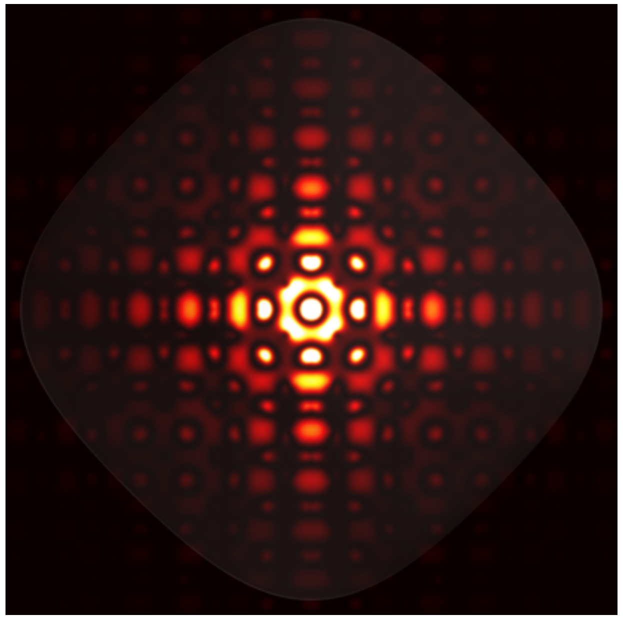
[Gao, et al. J. Appl. Phys. 114, 164302 (2013)]

Atomistic tight-binding



[Salfi, et al. Nat. Mat. 13, 605-610 (2014)]

Effective mass theory



[Gamble & Jacobson, et al. PRB **91**, 235318 (2015)]

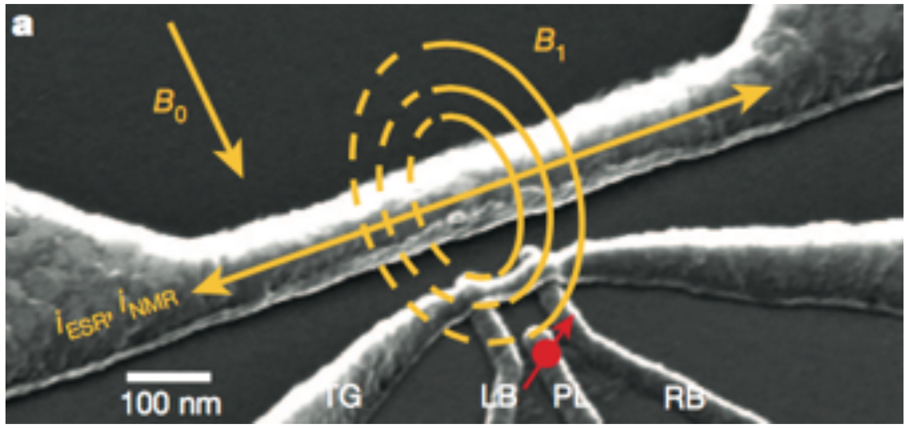
We identify “hot spots” with statistically stable tunnel coupling

Accept:
0.1 meV < t < 2 meV

Max prob.:
0.93 at 10 nm along [110]

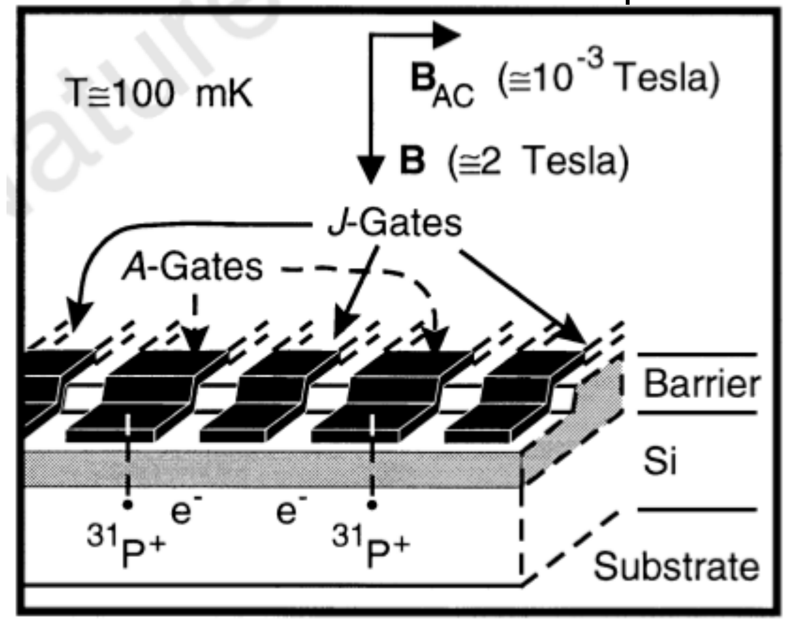
Straggle:
1 nm isotropic gaussian

Donor qubits in semiconductor systems



J. Pla, *et al.*, Nature (2013).

Electrons bound to impurities



Bruce Kane, Nature (1998).

- Kane quantum computer uses phosphorus donors in silicon as qubits.
- Like hydrogen atoms, except fixed in place in the crystal.
- Experimentally demonstrated!
- But the electronic structure of silicon is complicated…

Question: Can we couple two donor qubits together?

Answer: Probably not, at least not with high probability.

Interface roughness strongly affects valley splitting.

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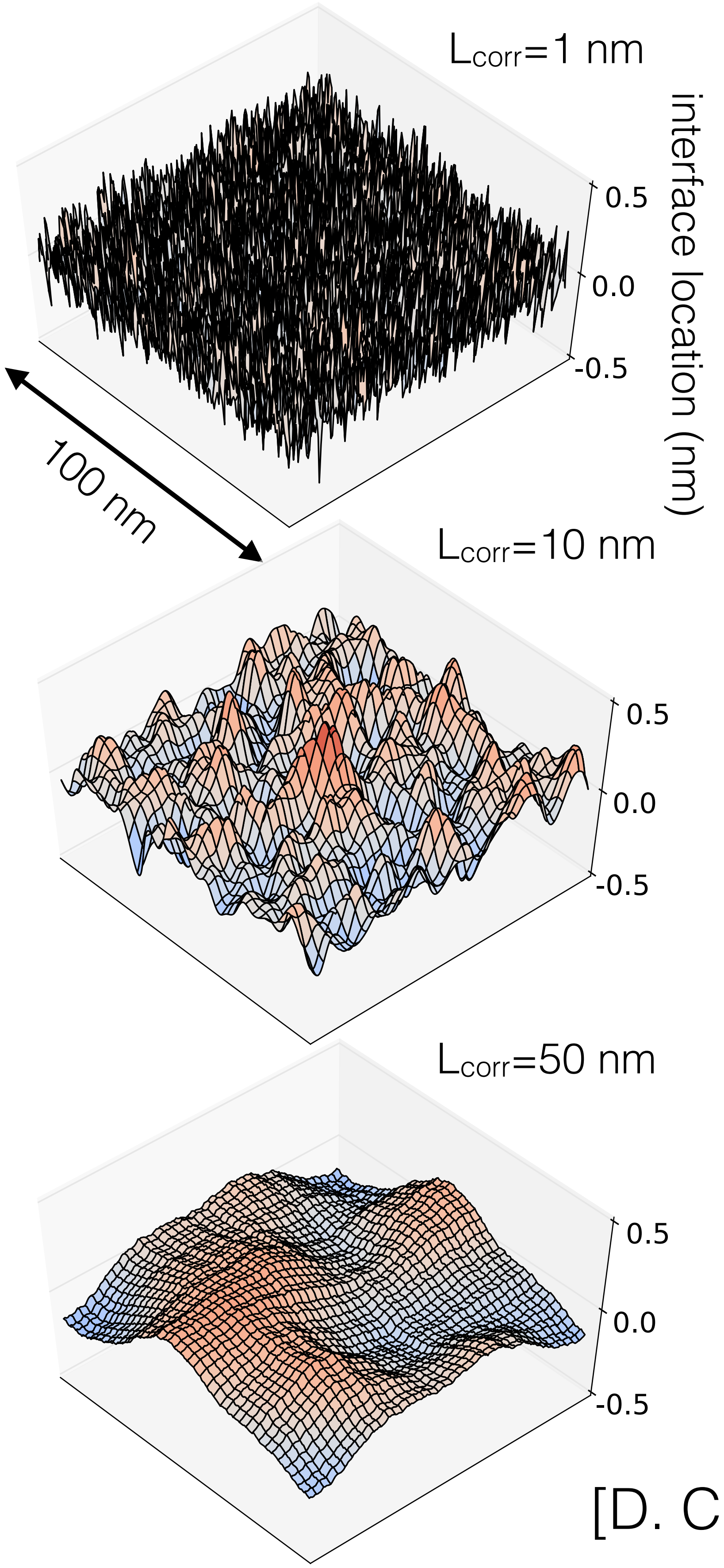
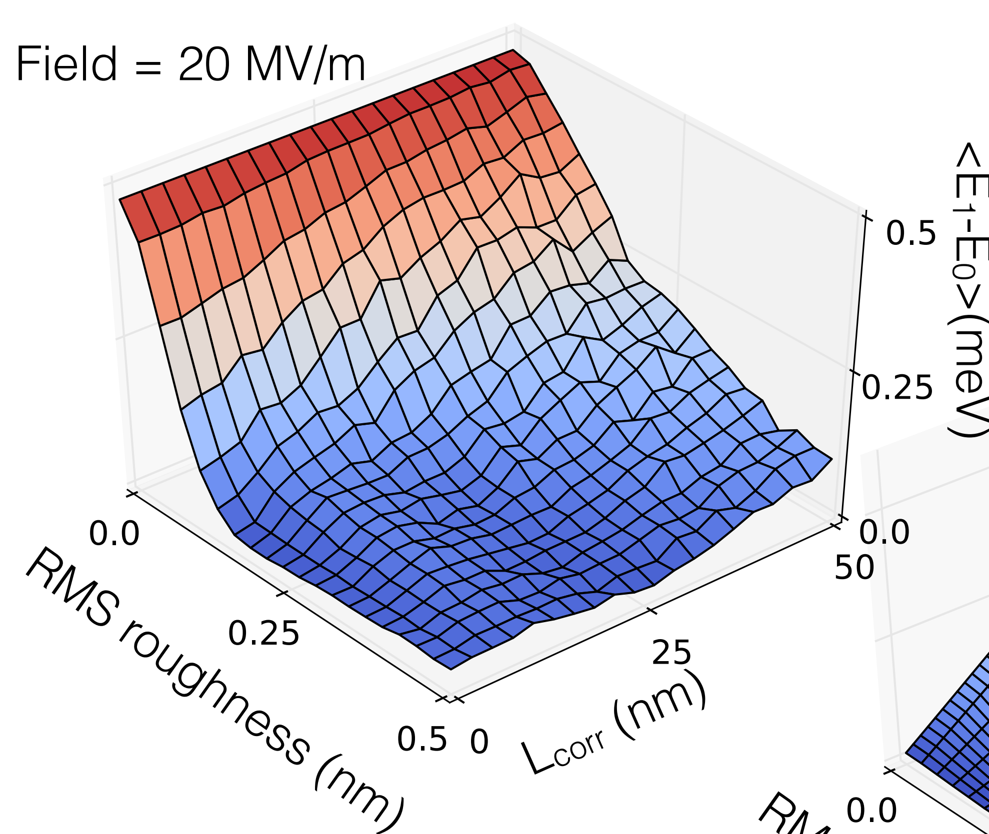
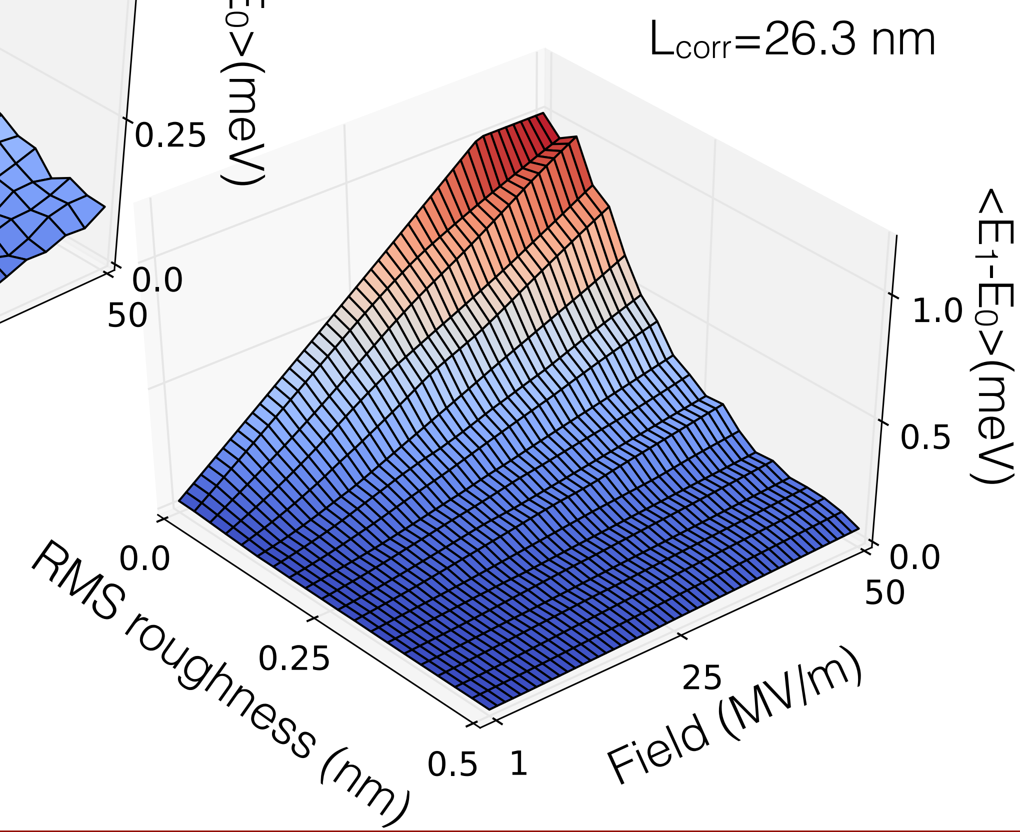


- We simulate rough interfaces by sampling random cases parameterized by RMS roughness and correlation length.
- We have:
  - 20x20 grid of roughness parameters
  - 65 disorder realizations each
  - ~100 voltage + offset configurations
- = 2.6 million **non-perturbative** calculations.





[D. Culcer *et al.* PRB (2010)].

Realistic interface roughness is consistent with observed valley splitting.