NEMO5

PhD Final Examination

Design and optimization of donor-based spin qubits in silicon

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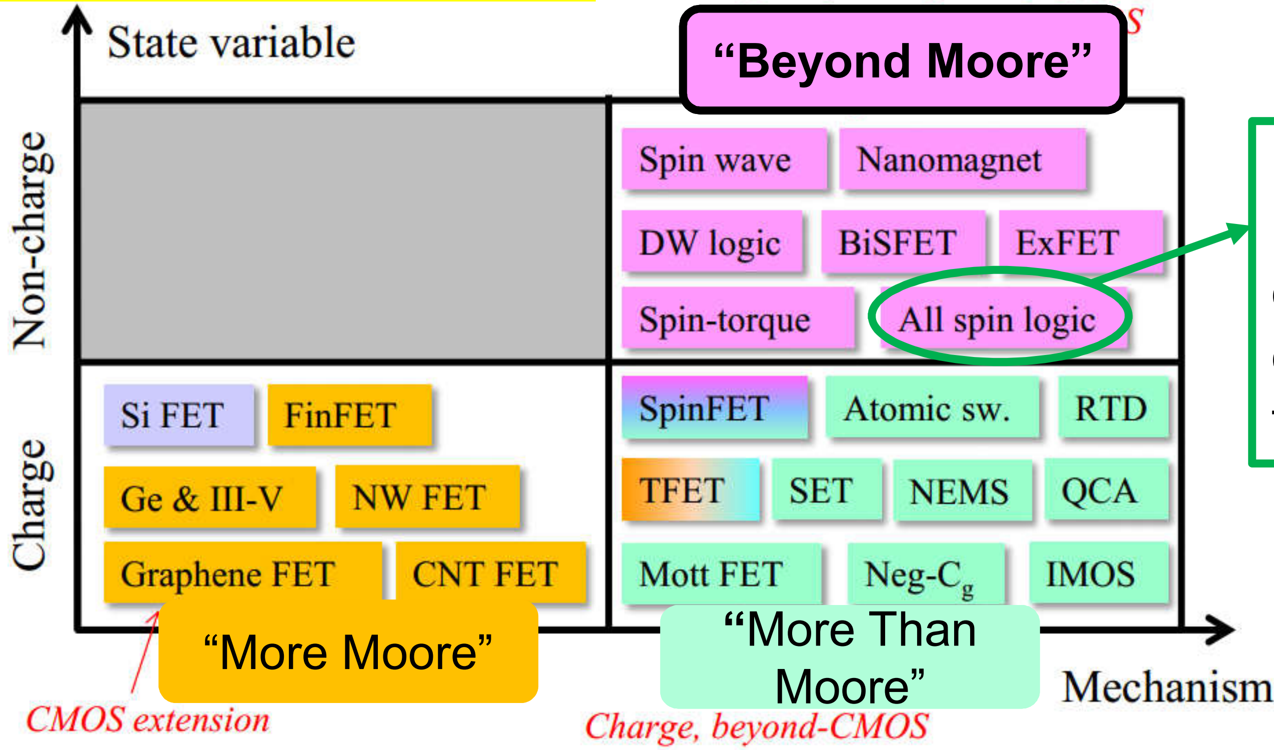
"Beyond Moore": quantum spin logic

Emerging logic devices



Quantum spin logic -- massive parallelism in quantum mechanics: 30 qubits more powerful than a supercomputer!

http://computer.howstuffworks.com/quantum-computer1.htm

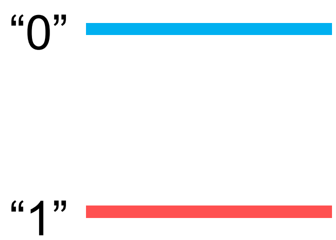
A. Chen, IEEE International Conference on IC Design & Technology, Pg. 1-4 (2014).

http://docplayer.net/120178-On-the-convergences-between-more-moore-more-than-moore-and-beyond-cmos.html

Research area: quantum spin logic devices

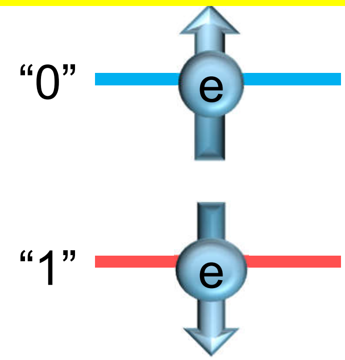
Basic units of quantum logic: qubits

Basic unit: quantum bit (qubit)



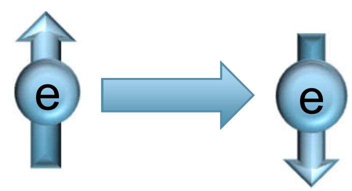
$$|Q\rangle = \alpha|0\rangle + \beta|1\rangle$$

Implementation



$$\alpha|\uparrow\rangle + \beta|\downarrow\rangle$$

Computing with quantum logic:



Number of qubits ↗ allowed functionalities ↗

Hardware: scalability is the key

- 4 qubits to factorize 143 (N. Xu et al., PRL 108, 130501 (2012))
- 30 qubits can outperform a classical computer (~3 billion transistors). http://computer.howstuffworks.com/quantum-computer1.htm

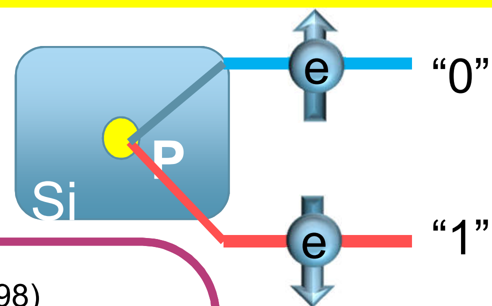
Allowed functionalities/Performance $\propto 2^N$

Realizing multi-qubit operations is the key

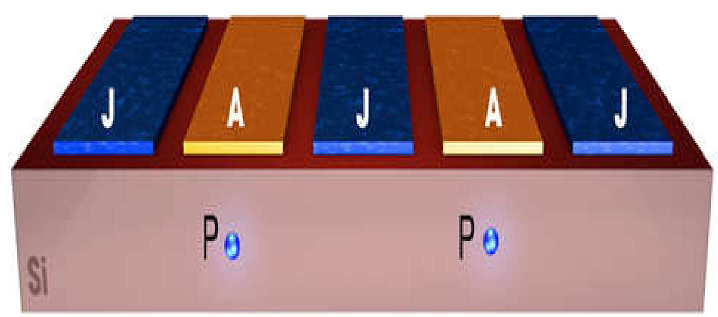
Hardware: scalability is the key

Focus: donor electron spin qubit

- Qubit implementation
- Architecture



Kane, Nature 393, 133 (1998)



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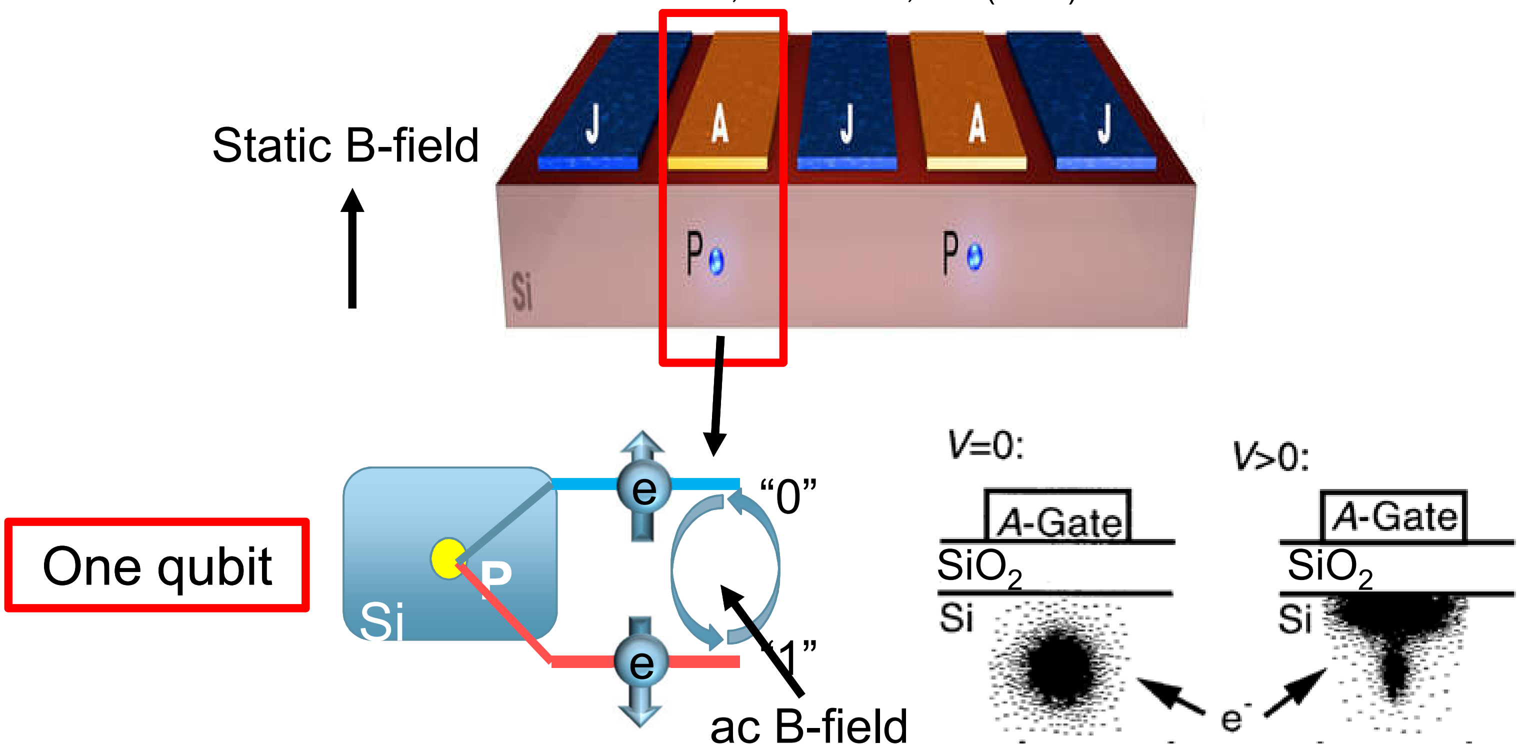
The popular Kane architecture: one qubit

Kane, Nature 393, 133 (1998)

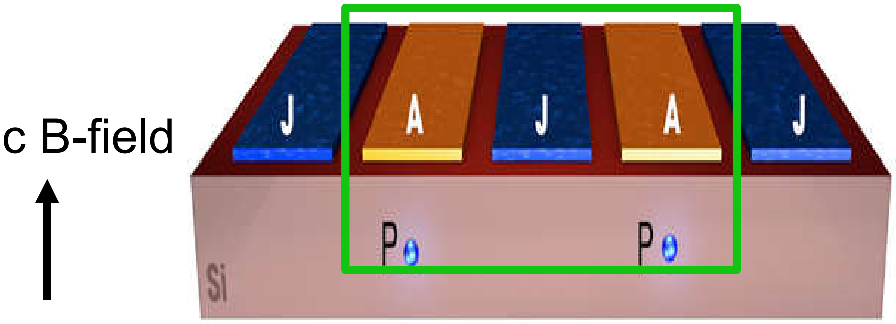


1-qubit control:
Gate controlled resonance frequency

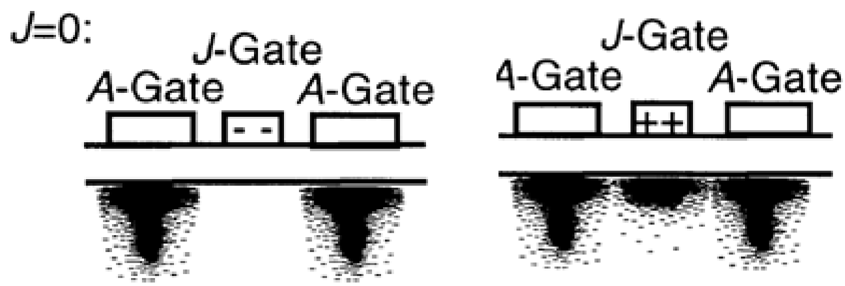
The popular Kane architecture: two qubits

Kane, Nature 393, 133 (1998)

Static B-field



Two qubits

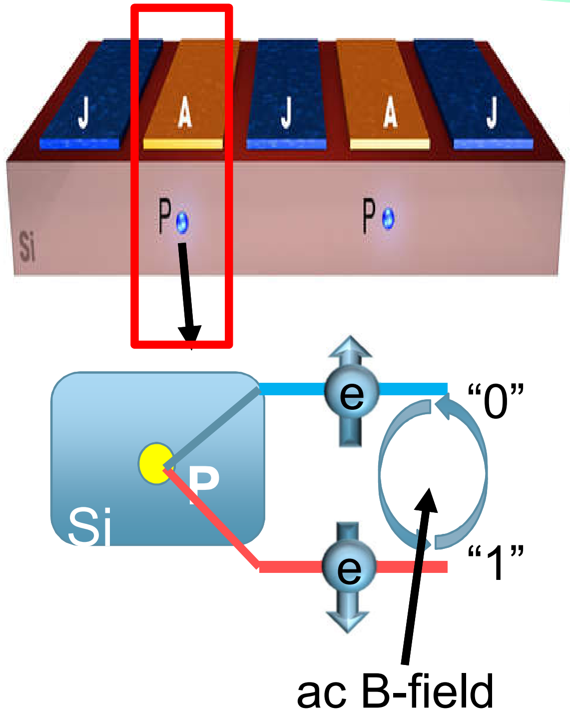


2-qubit control:
Exchange (J) ∝ wavefunction overlap

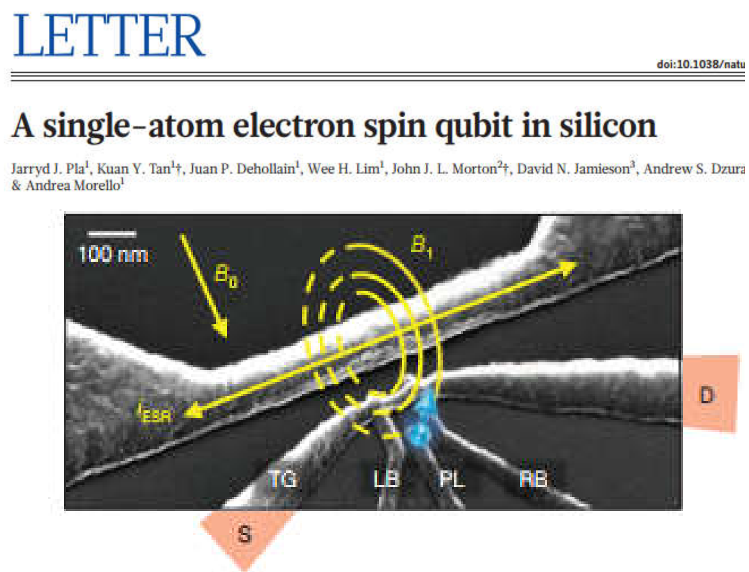
Efforts in experiment on Kane architecture?

Progress in donor-based quantum computing

1998 → 2012 → 2015



Kane, Nature 393, 133 (1998)

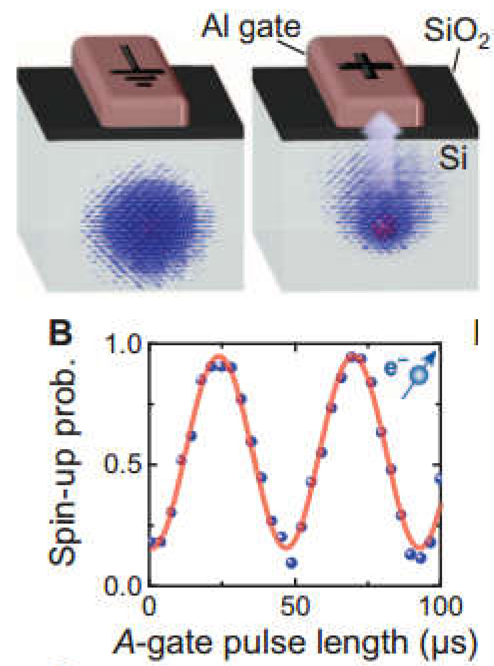

LETTER

doi:10.1038/natu

A single-atom electron spin qubit in silicon

Jarryd J. Pla[1], Kuan Y. Tan[1]†, Juan P. Dehollain[1], Wee H. Lim[1], John J. L. Morton[2]†, David N. Jamieson[3], Andrew S. Dzura & Andrea Morello[1]

Pla et al., Nature 489, 541 (2012)



Laucht et al., Sci. Adv. 10 (2015)

✓ Single qubit

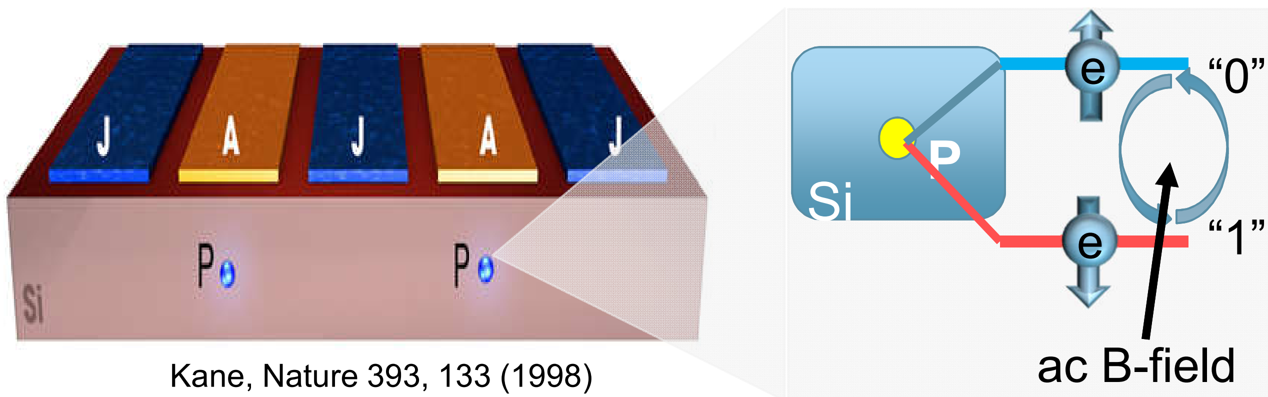
However, multiple-qubit operations haven't been realized. What is preventing us?

Challenges to realiz **multiple-qubit** operations using Kane architecture

Fabrication

Magnetic control (single qubit)

Exchange control (2 qubits)



Kane, Nature 393, 133 (1998)

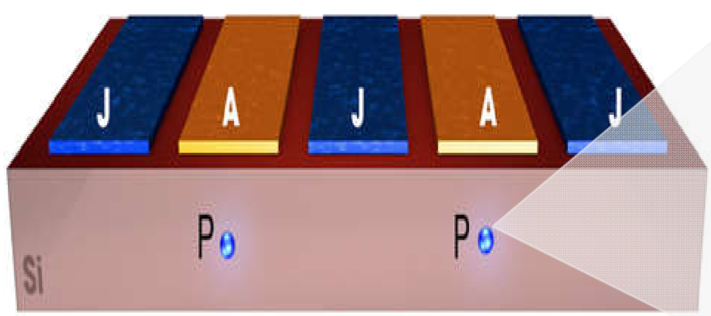
Challenges of Kane architecture

Challenges of realizing **multiple-qubit** operations using Kane architecture

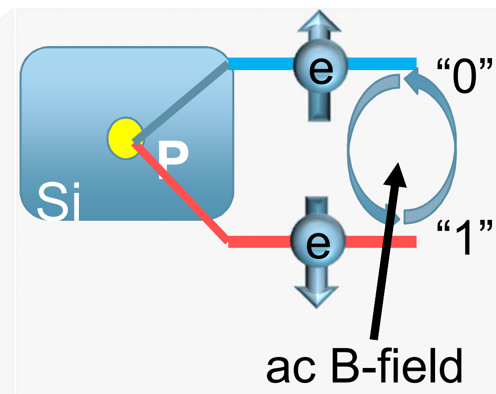
Fabrication

Magnetic control (single qubit)

Exchange control (2 qubits)

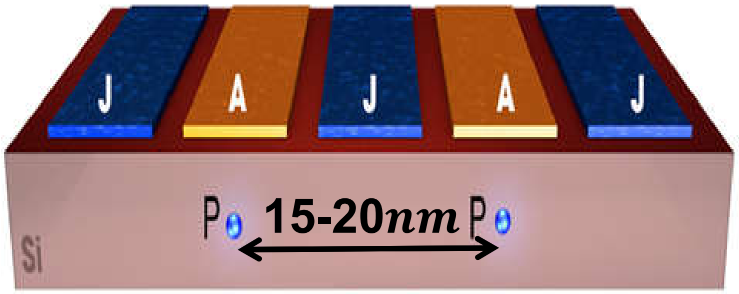


Kane, Nature 393, 133 (1998)



Challenge1 of Kane architecture: High gate density

Kane, Nature 393, 133 (1998).



Fabrication challenge

pack 3 gates in an ultra small length scale

→ gate short and crosstalk

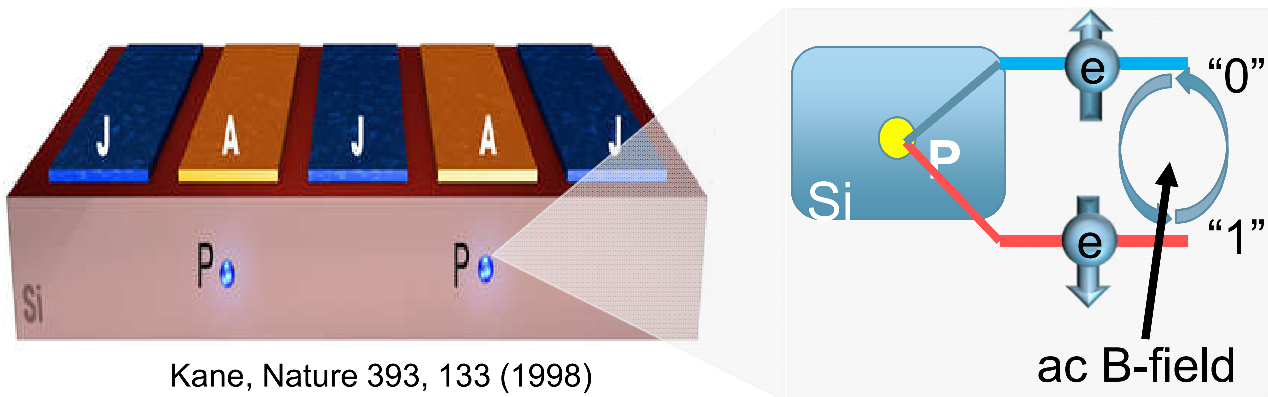
An alternative design with lower gate density is needed.

Challenges of realizing **multiple-qubit** operations using Kane architecture

Fabrication

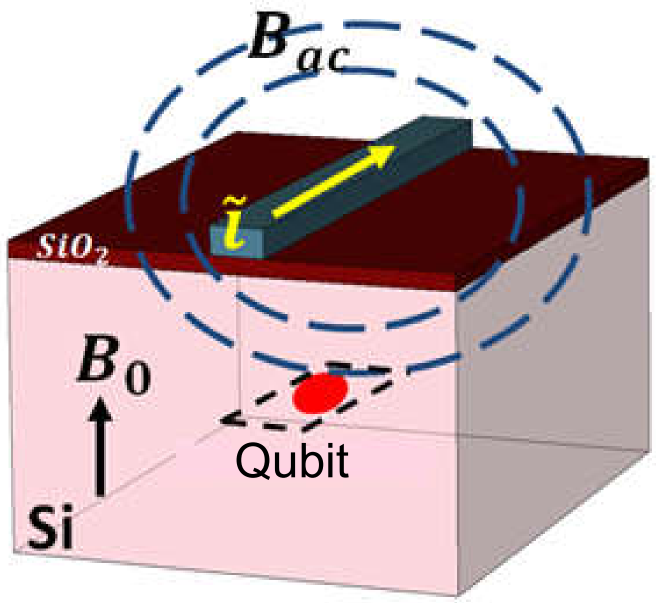
Magnetic control (single qubit)

Exchange control (2 qubits)

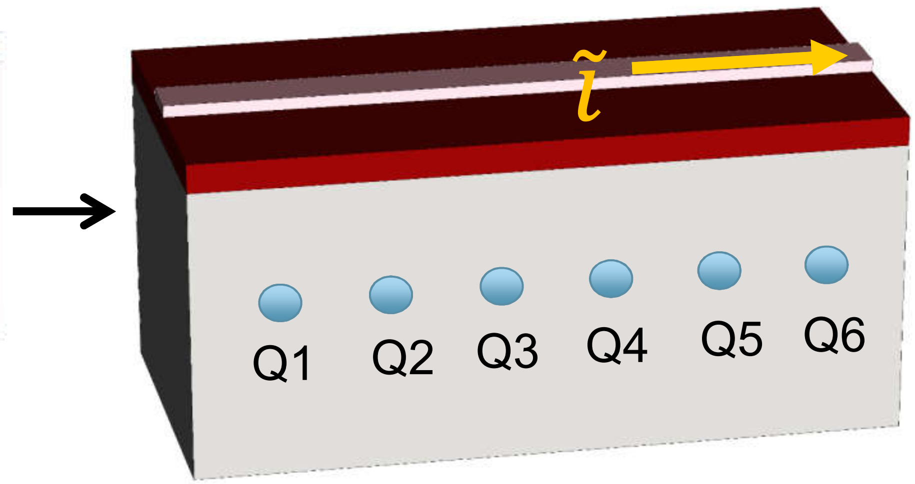


Kane, Nature 393, 133 (1998)

Challenge2 of Kane architecture: magnetic control



Scaled-up multiple qubits



Issues of magnetic control

- Difficult to apply local ac B-fields
- The metal wire introduces deleterious noise

J. Muhonen et al., Nature Nanotechnology 9, 986 (2014)

An alternative way to control spins locally is needed.

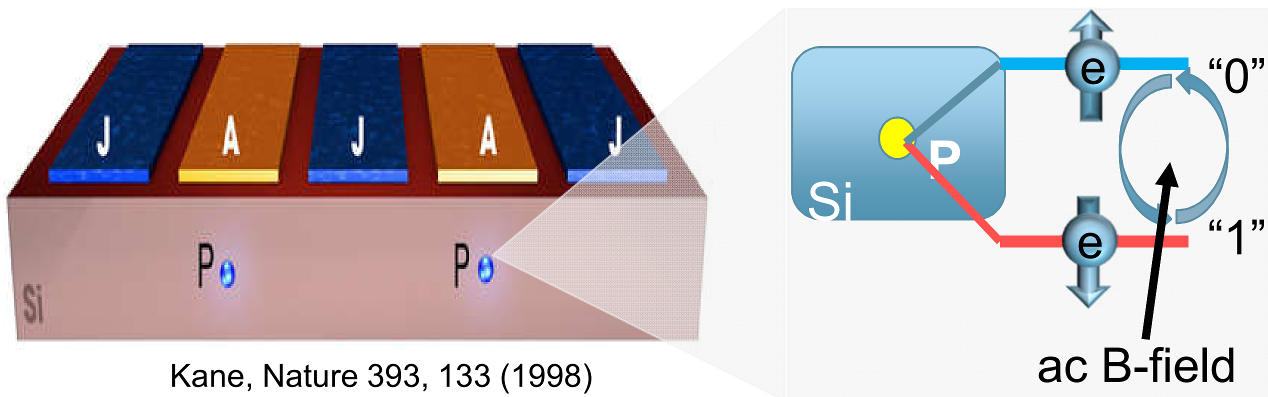
Challenges of Kane architecture

Challenges of realizing **multiple-qubit** operations using Kane architecture

Fabrication

Magnetic control (single qubit)

Exchange control (2 qubits)

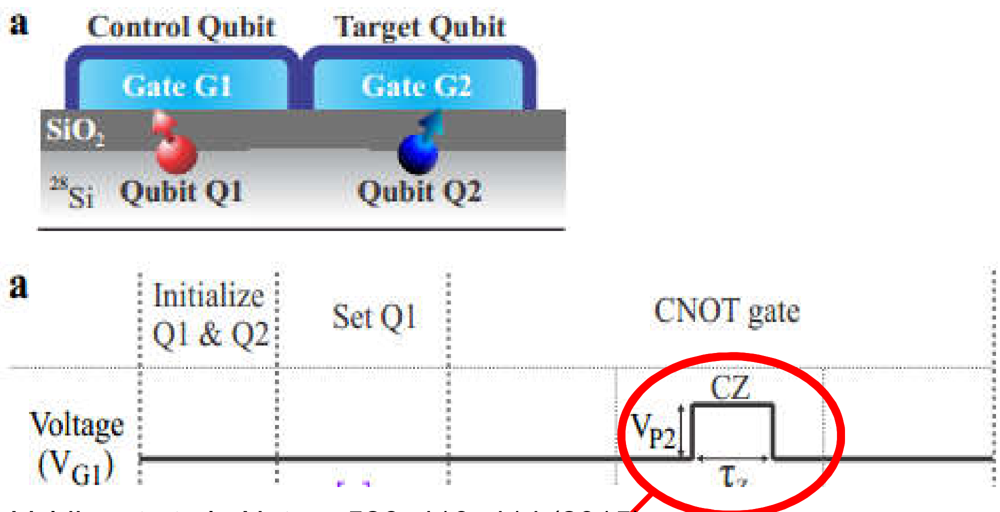


Kane, Nature 393, 133 (1998)

Ideal Exchange tunability

Key step in two-qubit operations: turn exchange on and off

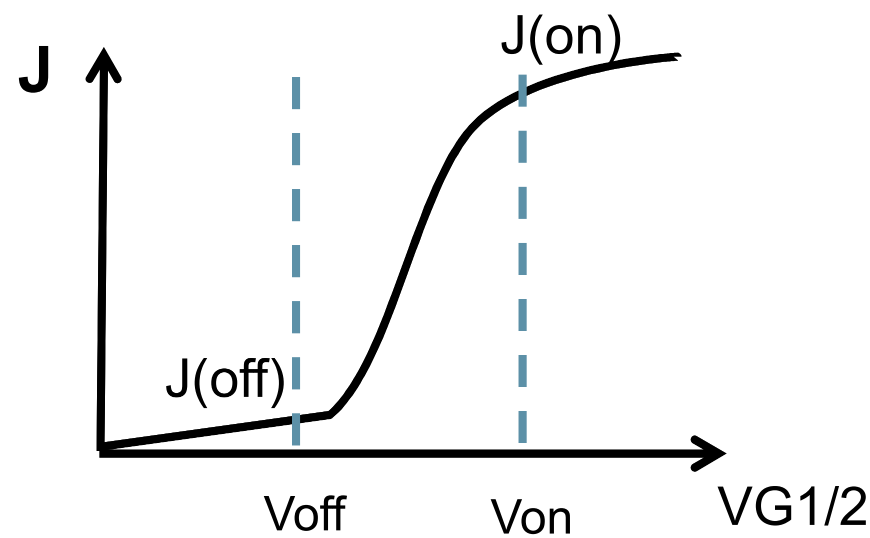
A two-qubit gate in double quantum dots



Veldhorst et al., Nature 526, 410–414 (2015)

One of the key factors to success: turn J on and off

Ideal tunability of J

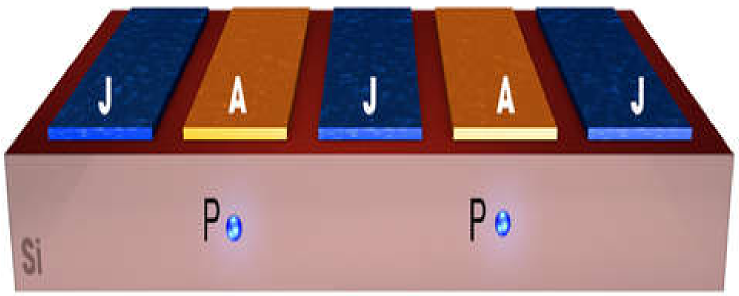


We need J(on) orders of magnitude larger than J(off).

Can this be achieved with Kane architecture?

Challenge3 of Kane architecture: exchange tunability

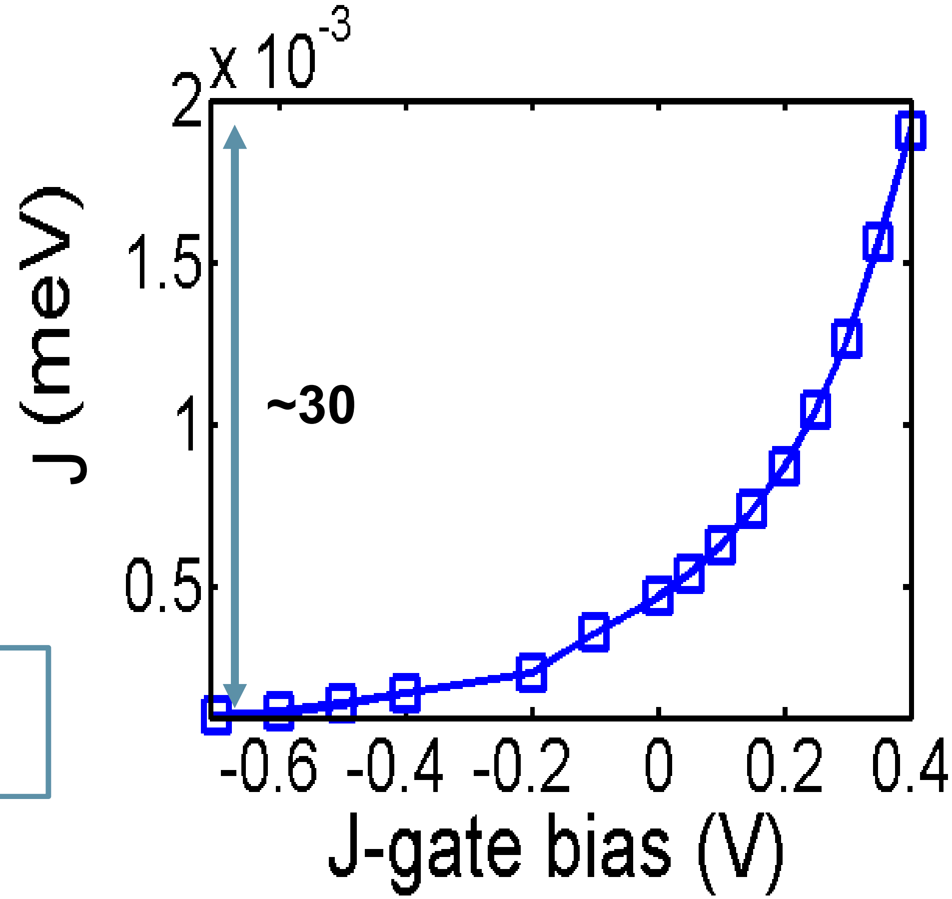
Kane J-gate



Kane, Nature 393, 133 (1998).

Limited J tunability:
J(on)/J(off) = ~30

Not enough to effectively turn the two-qubit operation on and off.

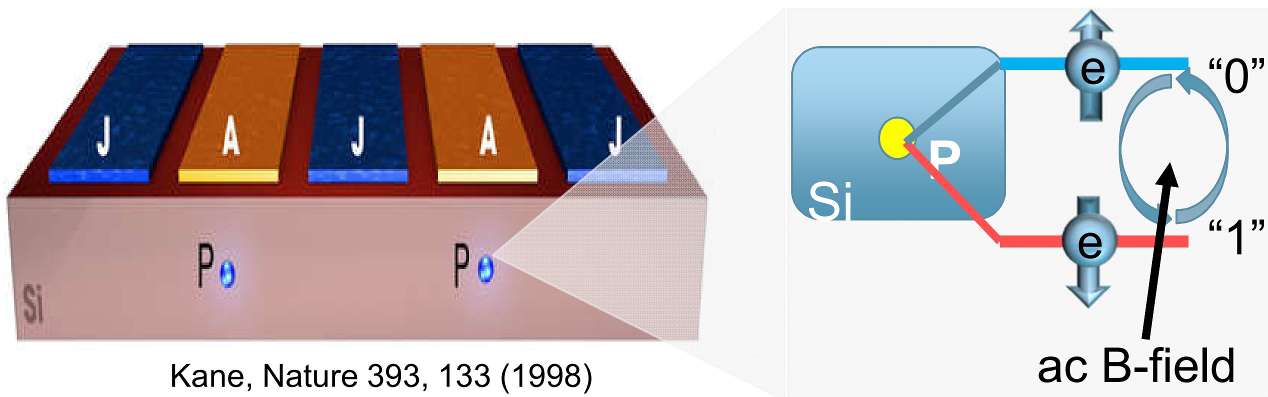


An alternative design that can provide enough J-tunability is needed.

Challenges of Kane architecture

Challenges of realizing **multiple-qubit** operations using Kane architecture

Gate density	Local control	J tunability
Fabrication	**Magnetic control (single qubit)**	**Exchange control (2 qubits)**



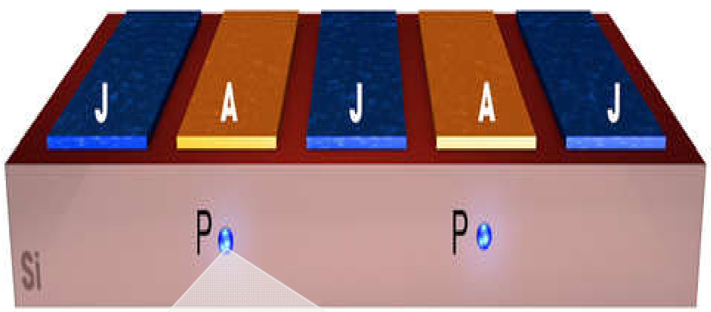
Kane, Nature 393, 133 (1998)

We need a design that could overcome all these challenges.

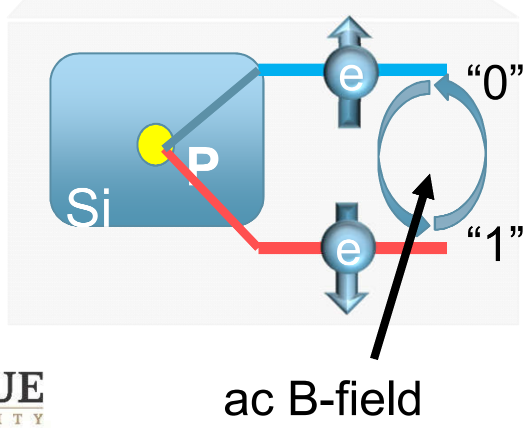
Proposed design: gate density and J tuning

Challenges to overcome

- ❑ High gate density
- ❑ Exchange tunability
- ❑ Magnetic control

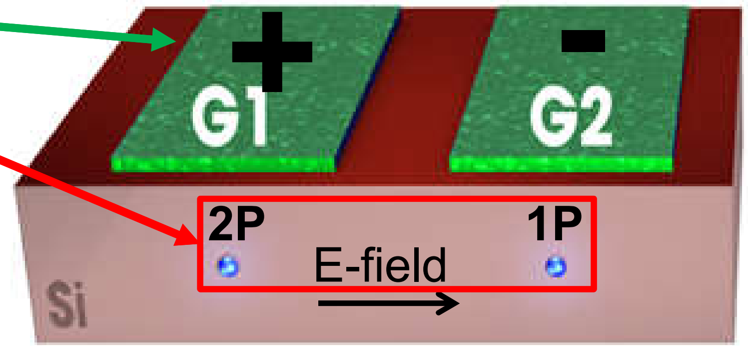


Kane, Nature 393, 133 (1998)

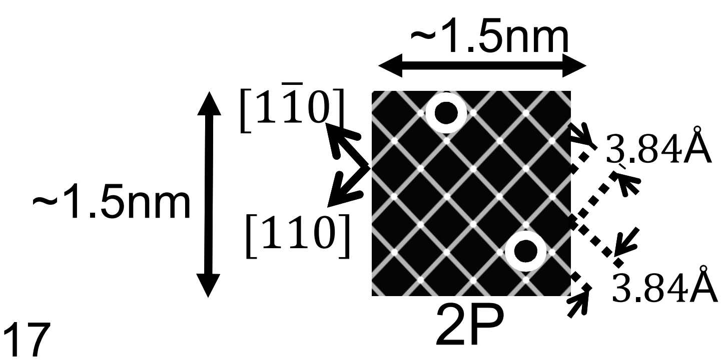


Proposed design

Wang et al., Nature Quantum Info. 2, 16008 (2016)



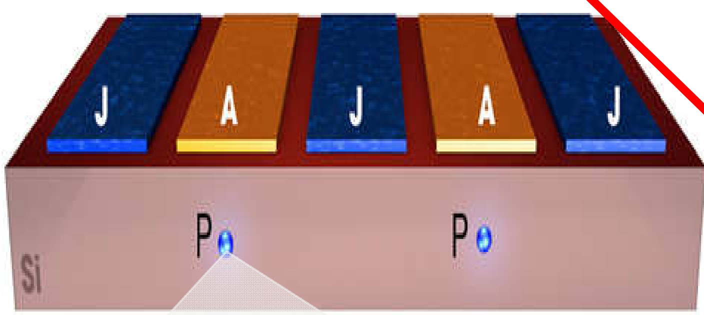
- Gate density is reduced by ~2.
- Exchange can still be tuned even without a J-gate.



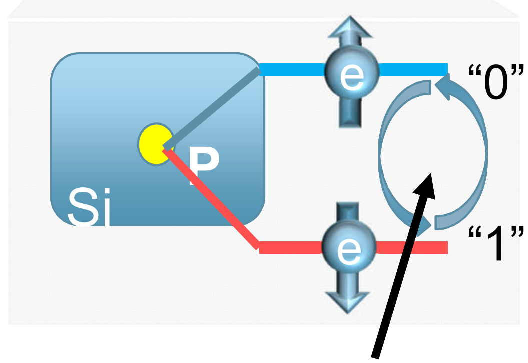
Proposed design: electrical control of spin

Challenges to overcome

- ❑ High gate density
- ❑ Exchange tunability
- ❑ Magnetic control

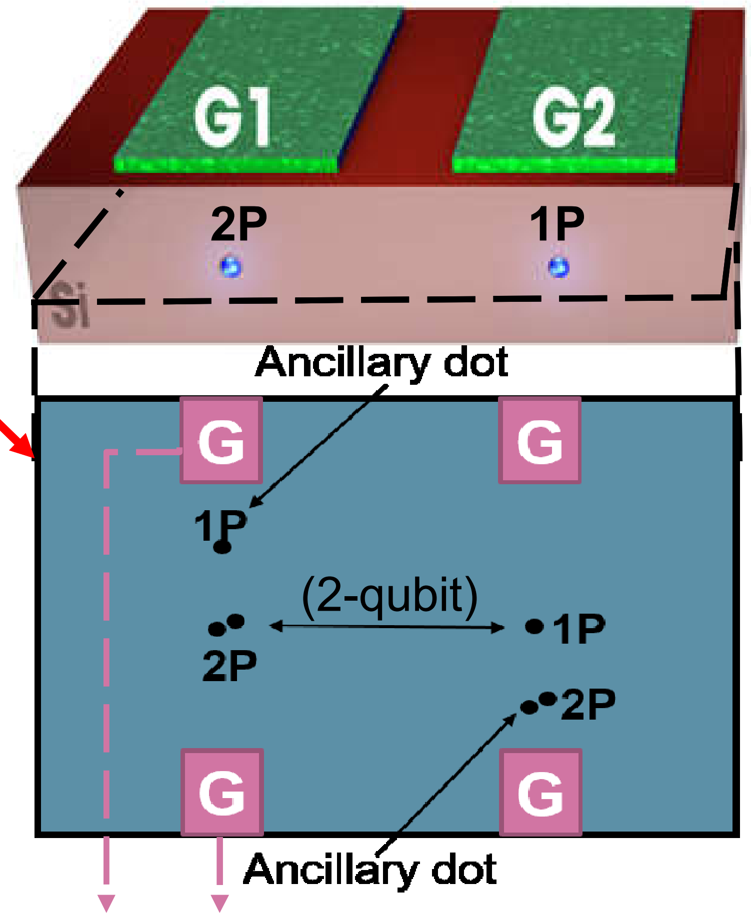


Kane, Nature 393, 133 (1998)



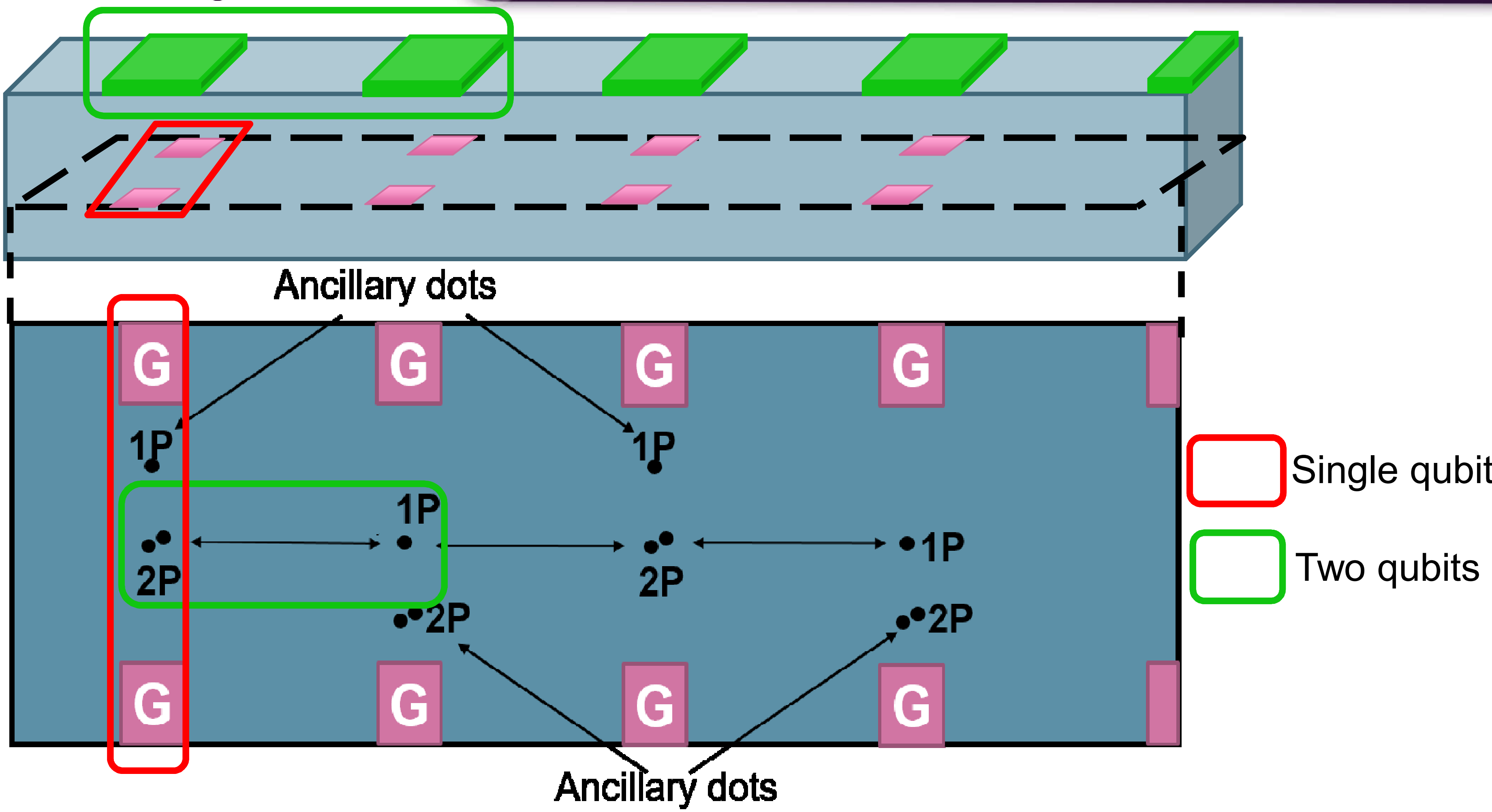
Proposed design

Wang et al., arXiv:1703.05370 (2017).



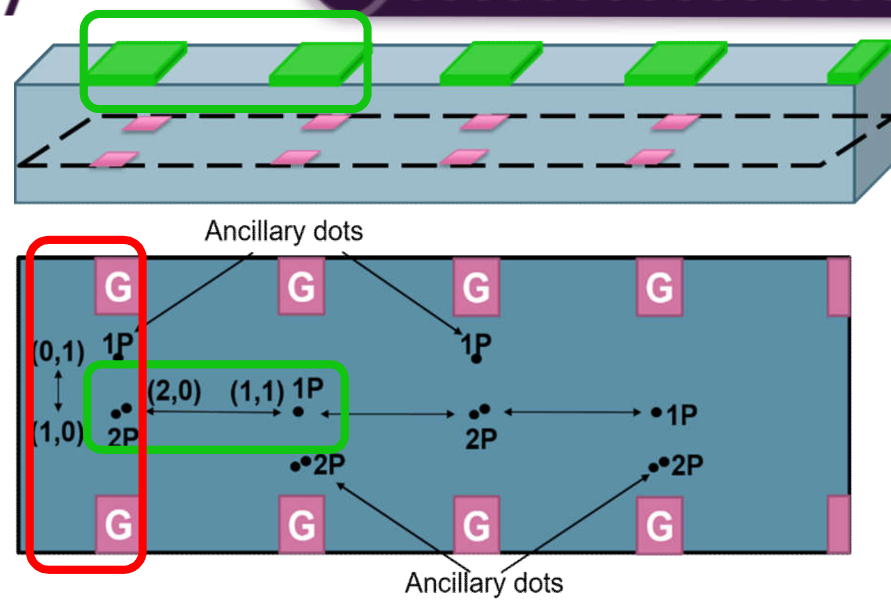
To achieve electrical control of spin qubits

Scalability of the proposed structure



Linear 1NN quantum computing: A. Fowler et al., Quant. Info. Comput. 4, 237-251 (2004)

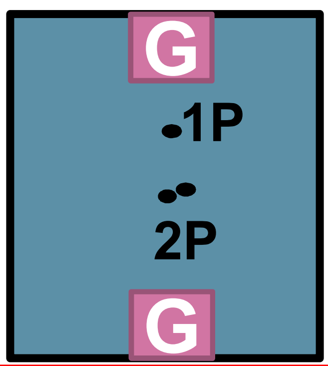
This device structure realizes all-electrical-control of spin and is potentially scalable.



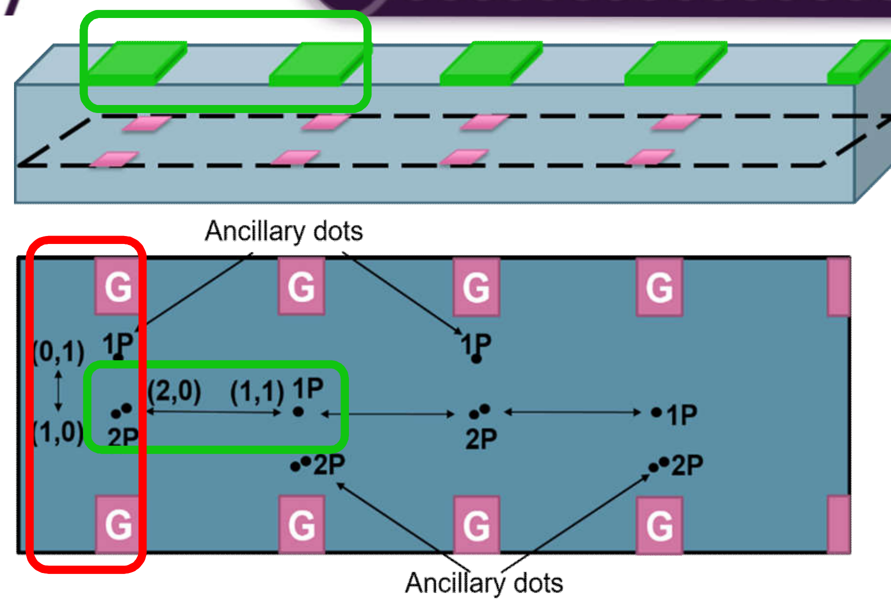
<u>Overcome challenges in Kane's architecture</u>

- √ Fabrication:
  - √ Gate separation
- √ All-electrical control
- √ Exchange tunability

All-electrical control of donor-based spin qubits



Engineering exchange coupling of two donor qubits



Overcome challenges in Kane's architecture

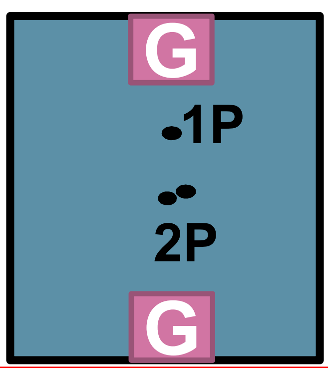
√ Fabrication:

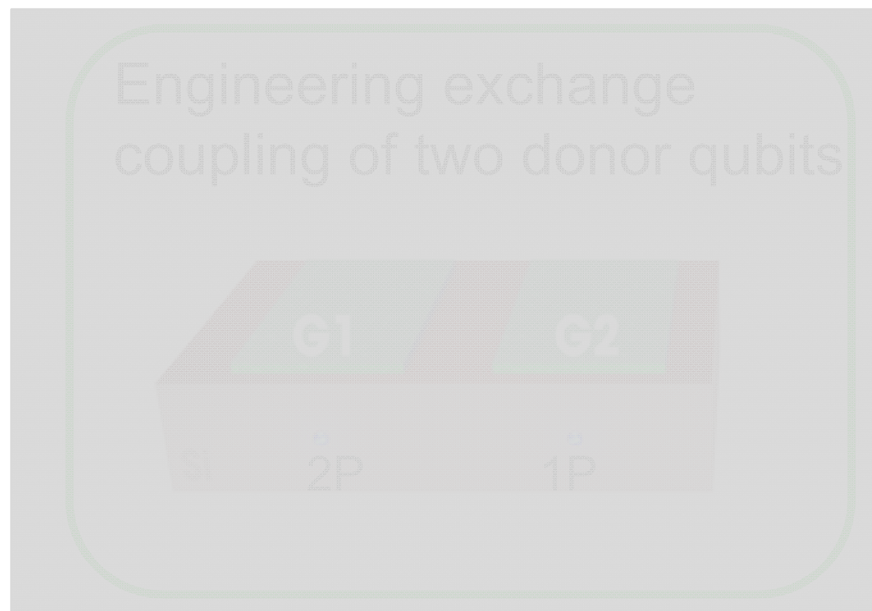
  √ Gate separation

√ All-electrical control

√ Exchange tunability

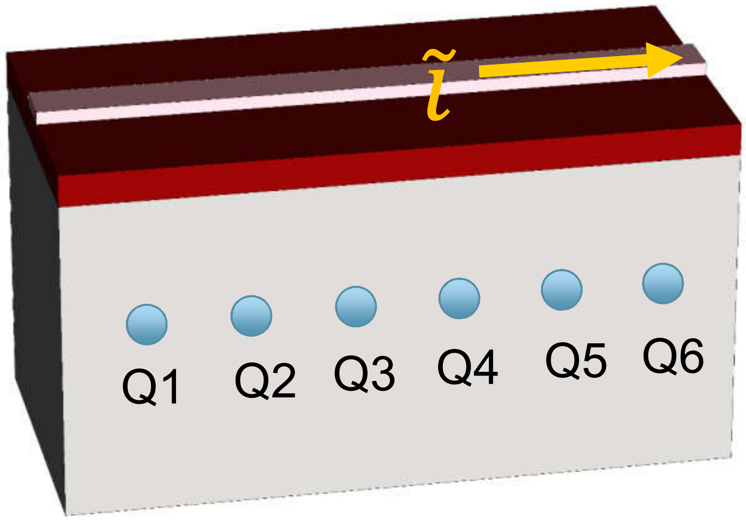
All-electrical control of donor-based spin qubits

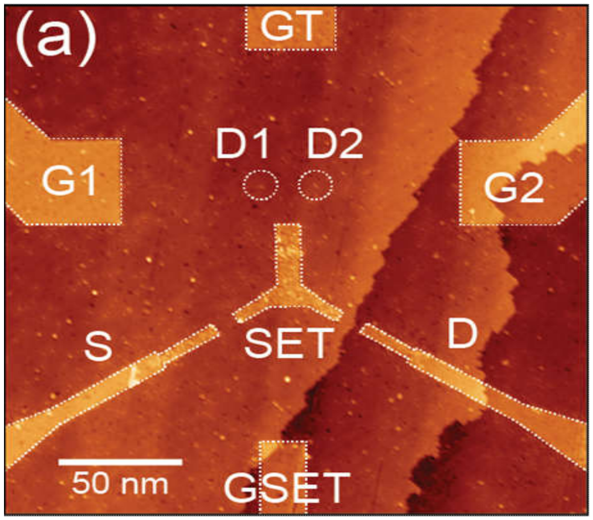




Electrical control of spins preferred

- Difficult to apply local ac magnetic fields.





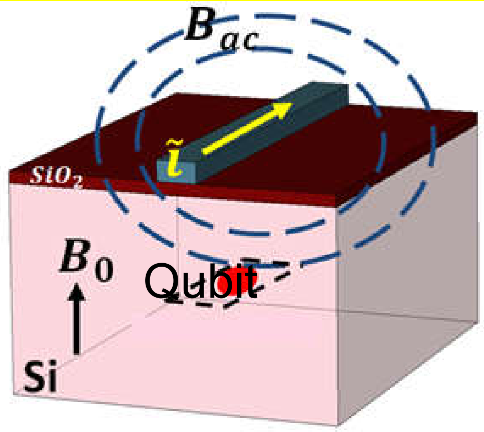
Watson et al., PRL 115, 166806 (2015).

- Applying localized, high-frequency electric fields is easier, and handy with existing circuitry.

- **Electrical control of spin qubits is more favorable.**
- **How to realize it?**

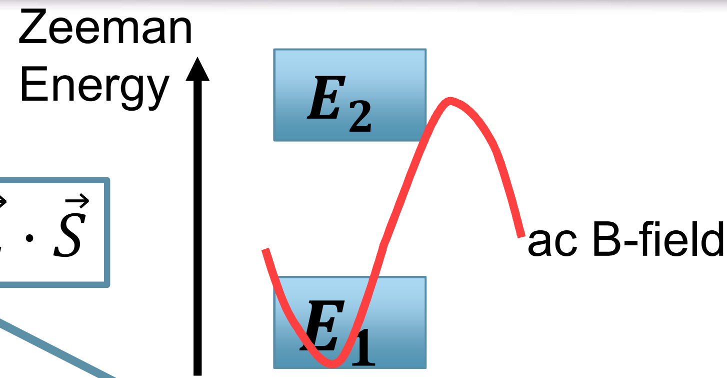
Electrical control of spin in quantum dots: local B-field difference + ac E-field

Spin control with time-varying B-field

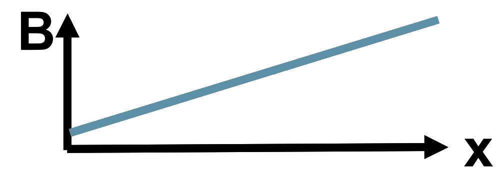


$$H = g\mu_B \overrightarrow{B_0} \cdot \vec{S} + g\mu_B \overrightarrow{B_{ac}} \cdot \vec{S}$$

$$\overrightarrow{B_{ac}} = \mathrm{b}_0 \sin(\omega t)$$



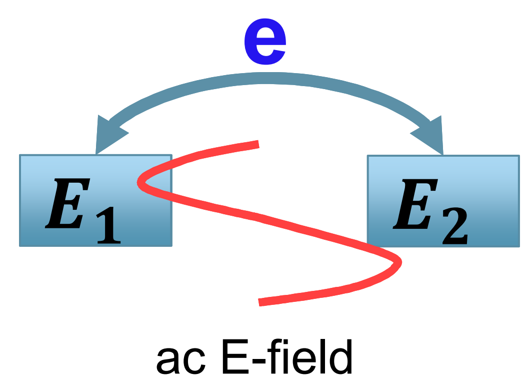
Spin control with spatially different B-field + ac E-field



LETTERS
PUBLISHED ONLINE: 10 AUGUST 2014 | DOI: 10.1038/NNANO.2014.153
nature nanotechnology

Electrical control of a long-lived spin qubit in a Si/SiGe quantum dot

E. Kawakami[1‡], P. Scarlino[1‡], D. R. Ward[2], F. R. Braakman[1†], D. E. Savage[2], M. G. Lagally[2], Mark Friesen[2], S. N. Coppersmith[2], M. A. Eriksson[2] and L. M. K. Vandersypen[1*]

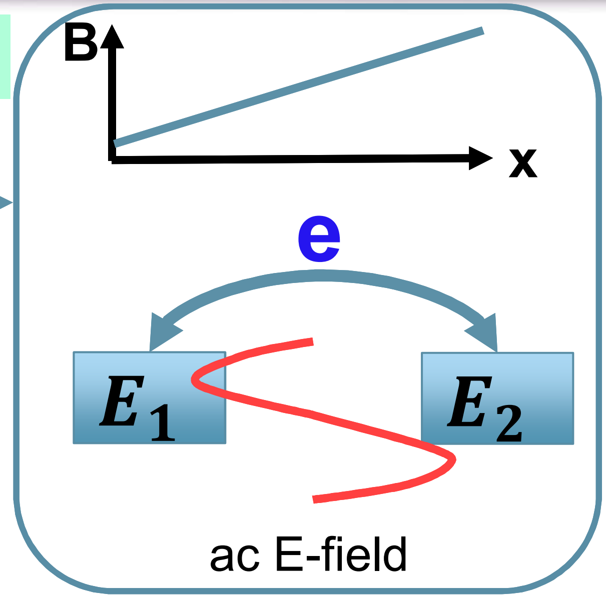


Spin rotation can be driven by ac E-field with local Zeeman energy difference.

Electrical control of spin in quantum dots: local hyperfine difference + ac E-field

Spin control with spatially different B-field + ac E-field

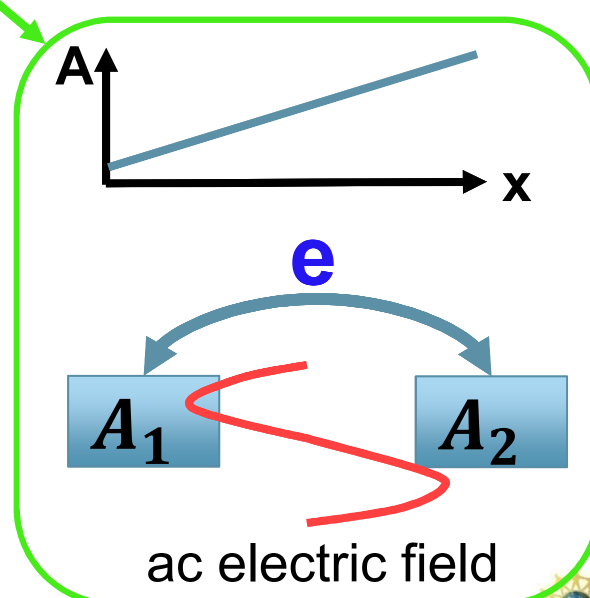
$$H = g\mu_B \overrightarrow{B_0} \cdot \vec{S} + g\mu_B \overrightarrow{B_{ac}} \cdot \vec{S}$$



Spin control with spatially different hyperfine couplings + ac E-field

$$H = g\mu_B \overrightarrow{B_0} \cdot \vec{S} + A\vec{I} \cdot \vec{S}$$

Introduces an effective B-field



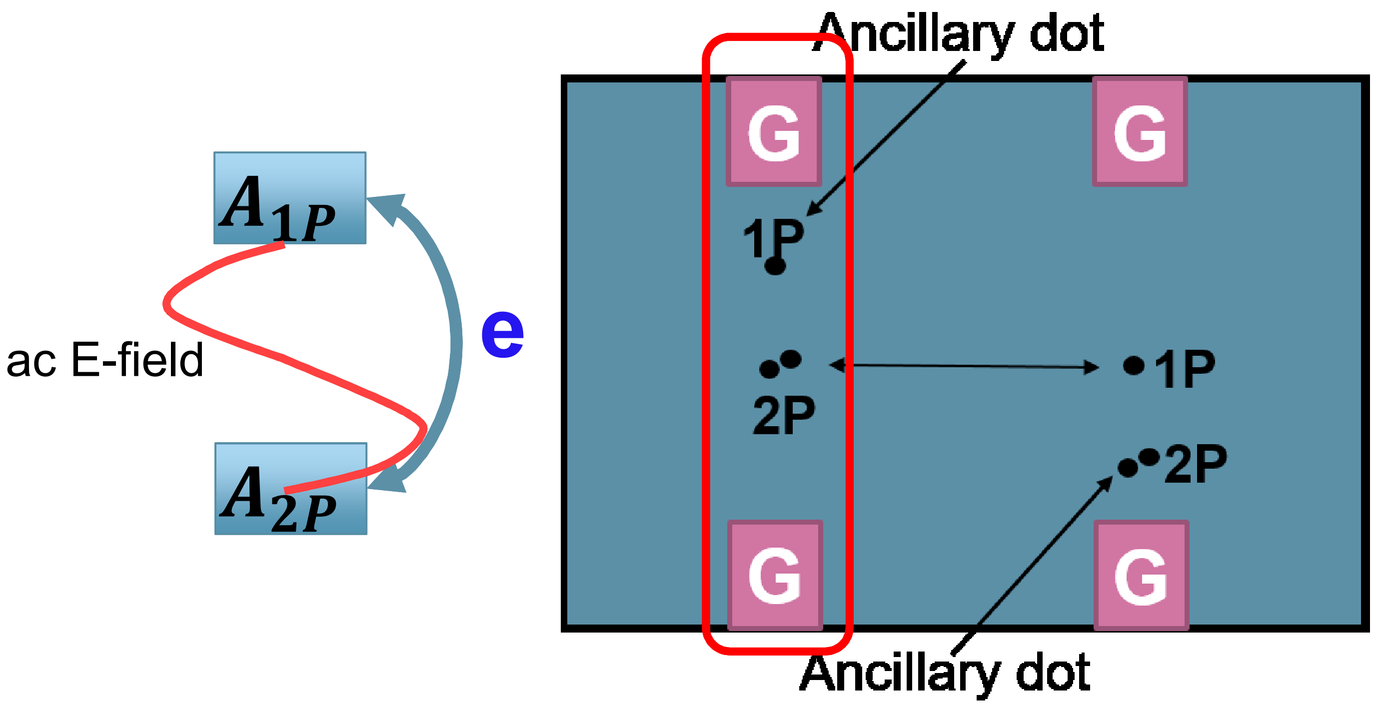
Effective ΔE_{Zeeman} can created by ΔA

Electron spin rotation can be driven electrically using spatially different hyperfine couplings.

In a QD system: Laird et al. PRL 99, 246001 (2007)

Electrical control of spin with ancillary donors

Introduce local hyperfine coupling difference with donors



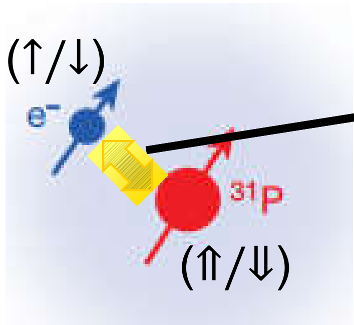
Modulation can be realized with the in-plane gates.

In principle, electrical control of electron spin can be realized in the proposed design.

Hyperfine interactions in 1P and 2P

J. J. Pla et al., Nature 489, 541-545 (2013)

1P

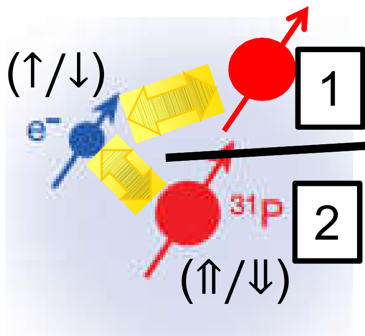


$A_{1P}\vec{I}\cdot\vec{S}$

N-spin e-spin

- A describes the strength of hyperfine interaction
- $A \propto |\Psi(at\ donor\ site)|^2$

2P



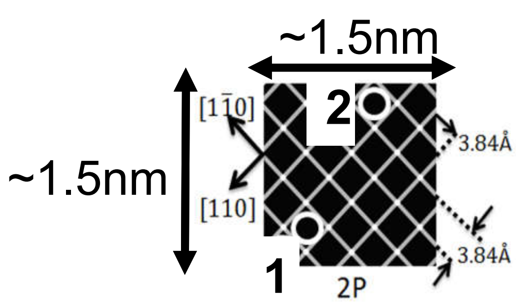
$A_{2P,1}\vec{I_1}\cdot\vec{S}$

$+A_{2P,2}\vec{I_2}\cdot\vec{S}$

A_{1P} and A_{2P} are different due to different quantum confinement

- $|\Psi(at\ donor\ site)|^2$ depends on E-field → A(E-field)

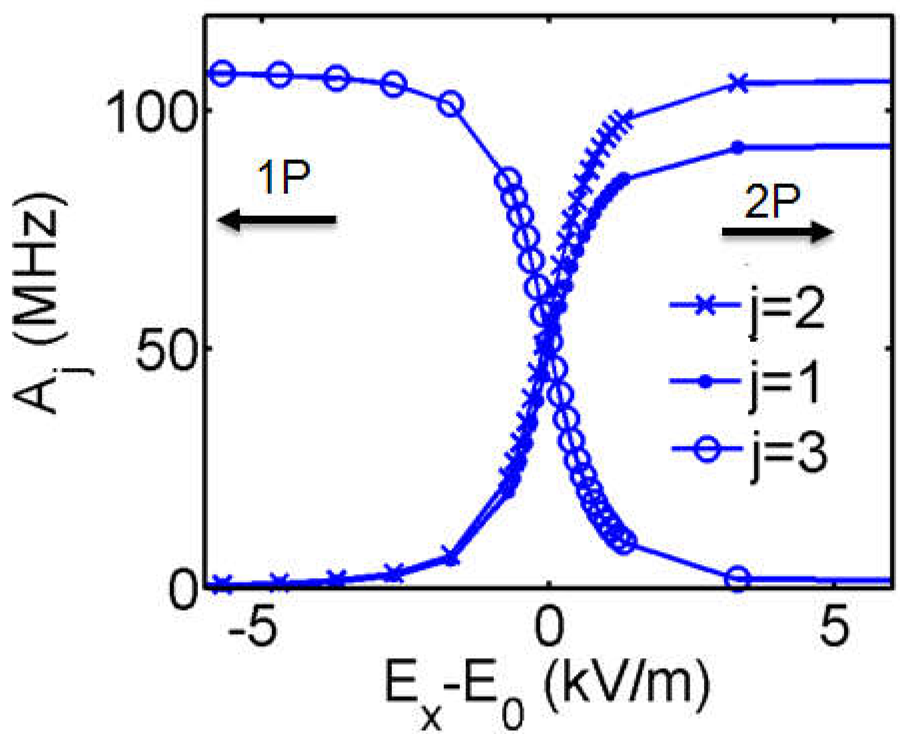
1. Rahman et al., PRL 99, 036403 (2007)



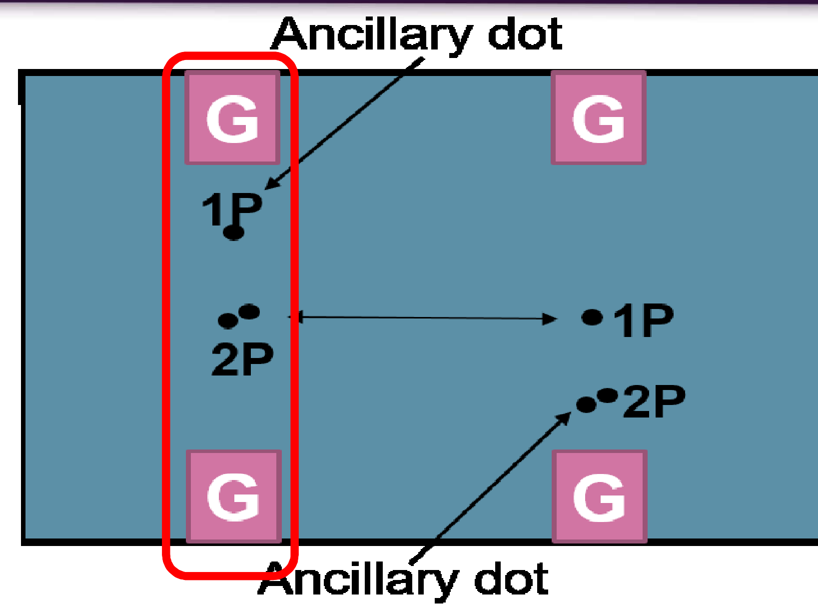
Utilize these for electrical control of spin.

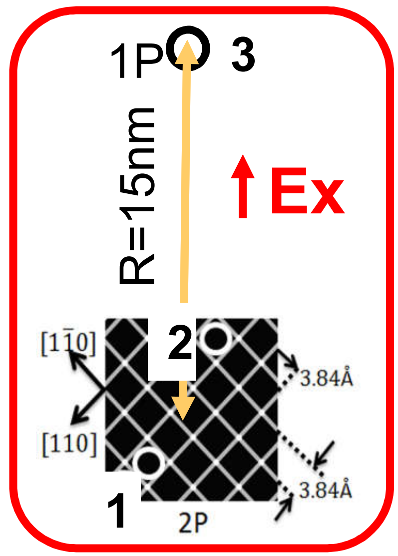
Tuning hyperfine coupling with E-fields

Hyperfine modulation in 2P-1P



(E_0 = -4.9634 MV/m)

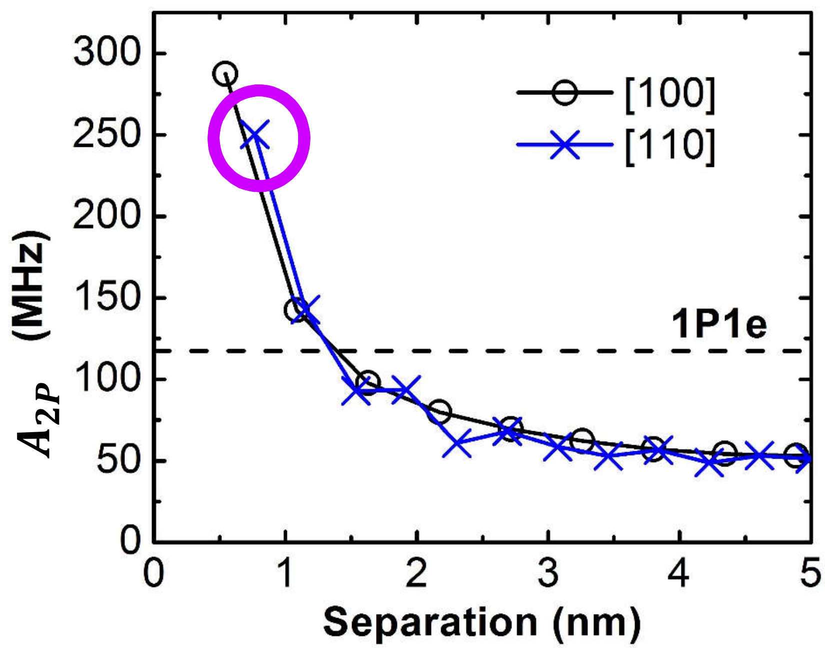




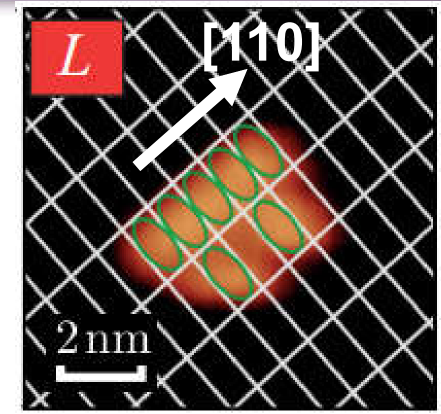
The hyperfine couplings can be modulated with electric fields.

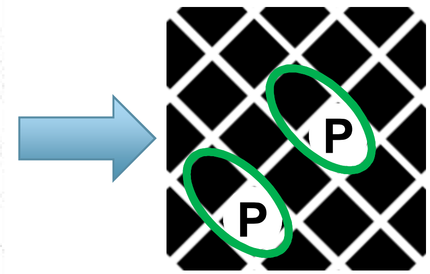
Experiment validation of 2P hyperfine

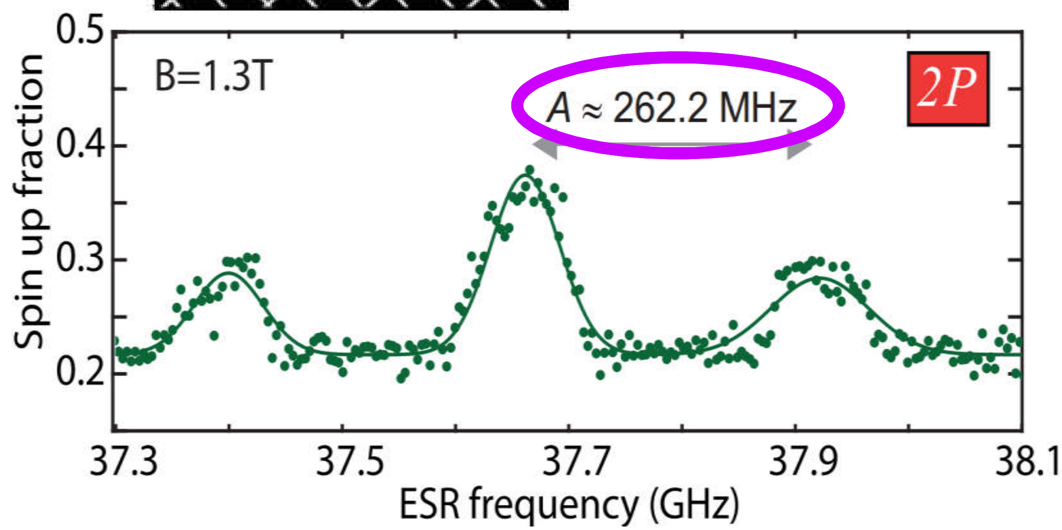
Metrology: mapping out 2P donor locations using hyperfine couplings.



Wang et al., Sci. Rep. 6, 31830 (2016)







(From Sam Hile, unpublished)

The hyperfine couplings in 2P agree with measurement.

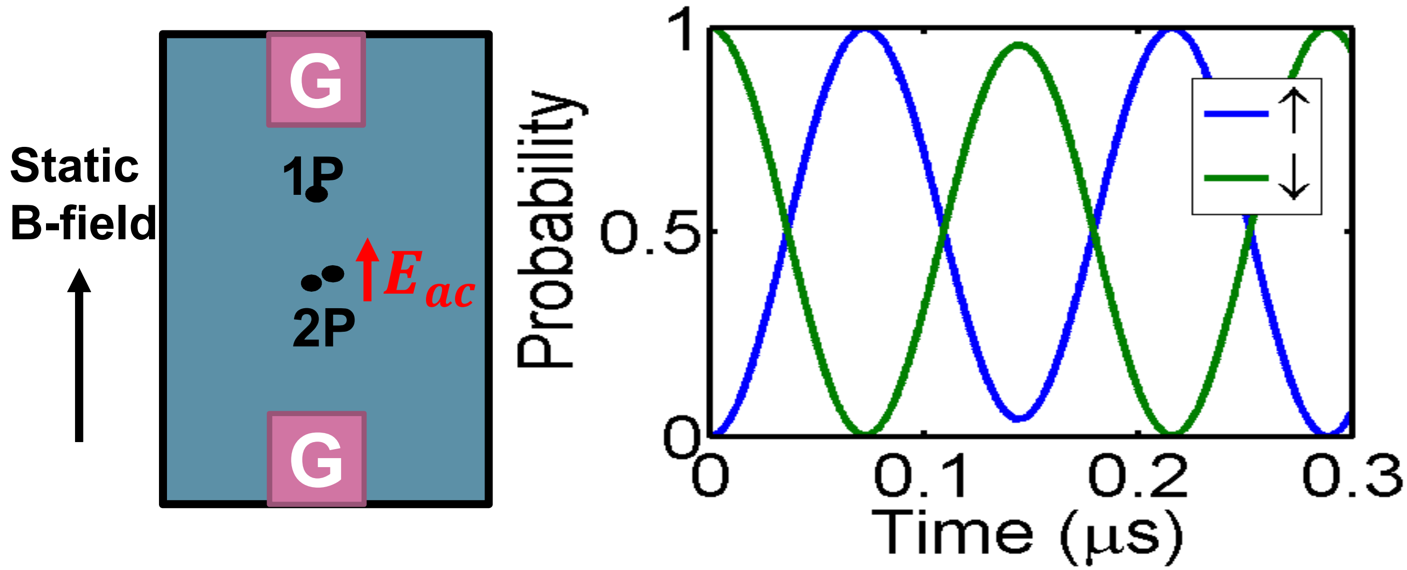
Spin evolution under ac E-field

Effective Hamiltonian describing the spin evolution

$$H = H_{Zeeman} + H_{hyperfine} + H_{tc} + H_{E_{ac}}$$

$+H_{tc}$: Allows charge transfer between 2P and 1P

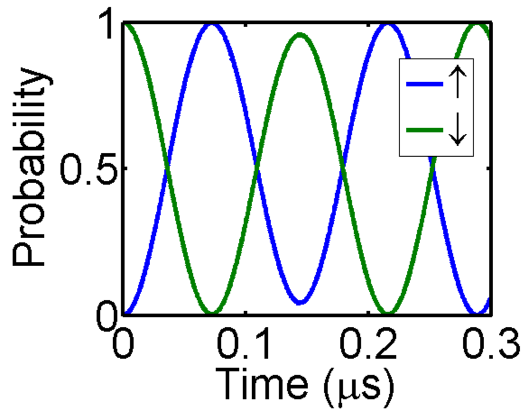
$+H_{E_{ac}}$: To drive the spin rotation



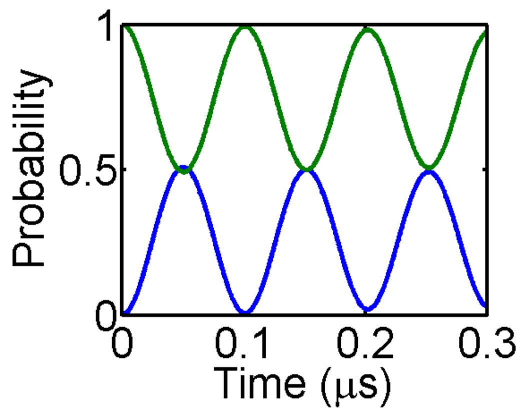
Electrical control of spin qubit can be realized with the proposed design.

Optimization of the 2P-1P qubit design

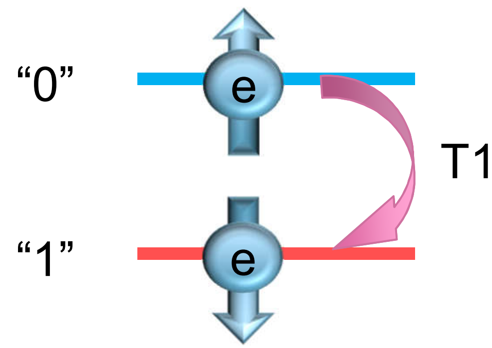
1. High control fidelity



vs

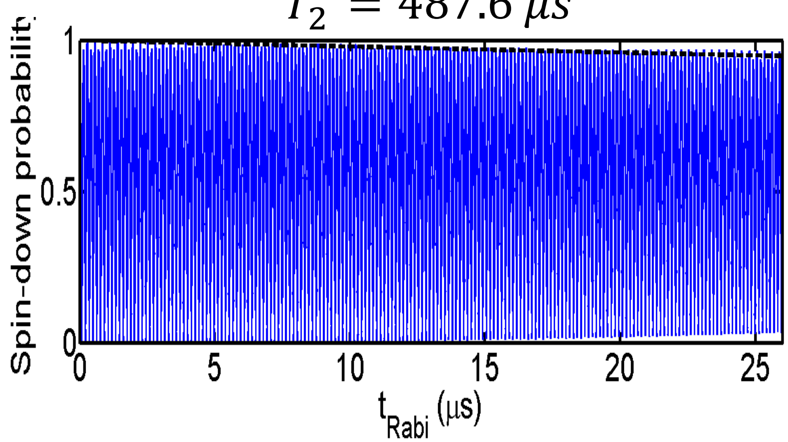


3. Long spin storage time (no operation)



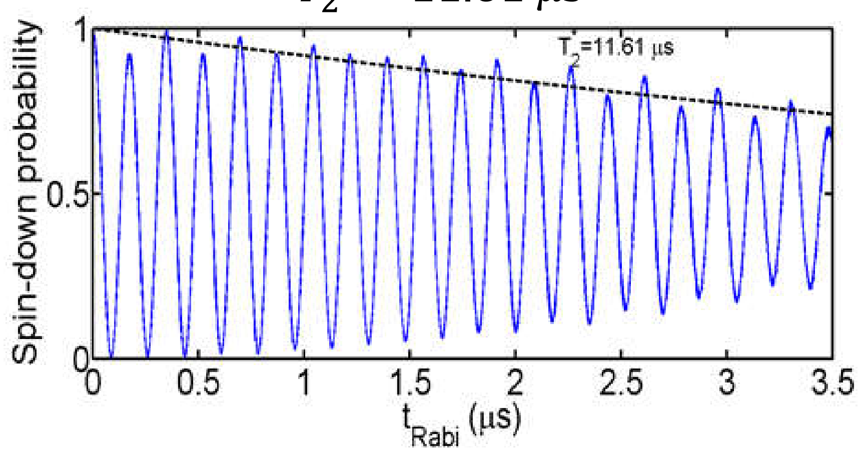
2. Long coherence time

$T_2^* = 487.6\ \mu s$

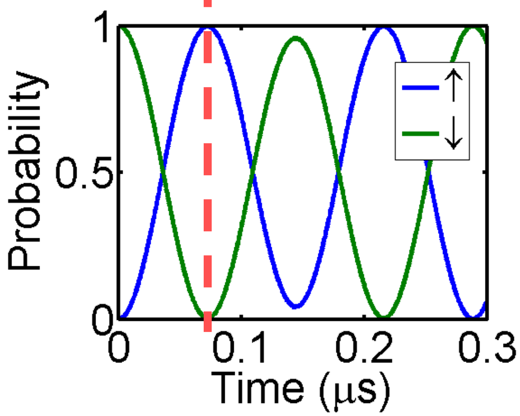


vs

$T_2^* = 11.61\ \mu s$

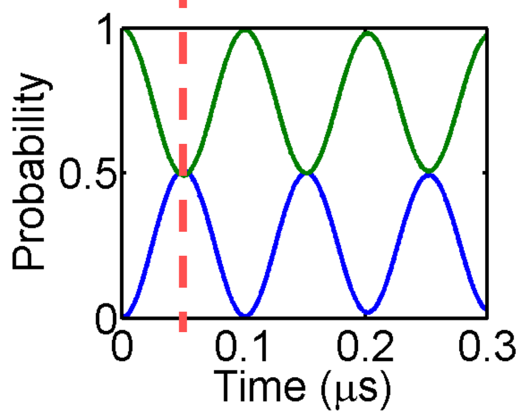


1. High control fidelity



~100%

vs

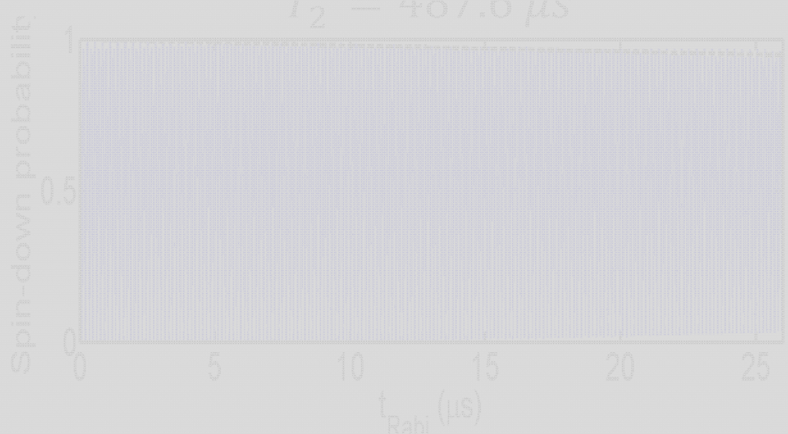


~50%

3. Long spin storage time (no operation)

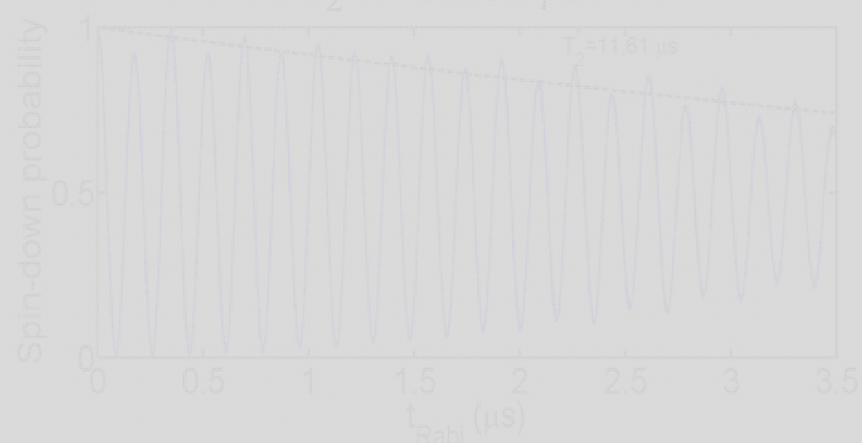
2. Long coherence time

$T_2^* = 487.6\ \mu s$



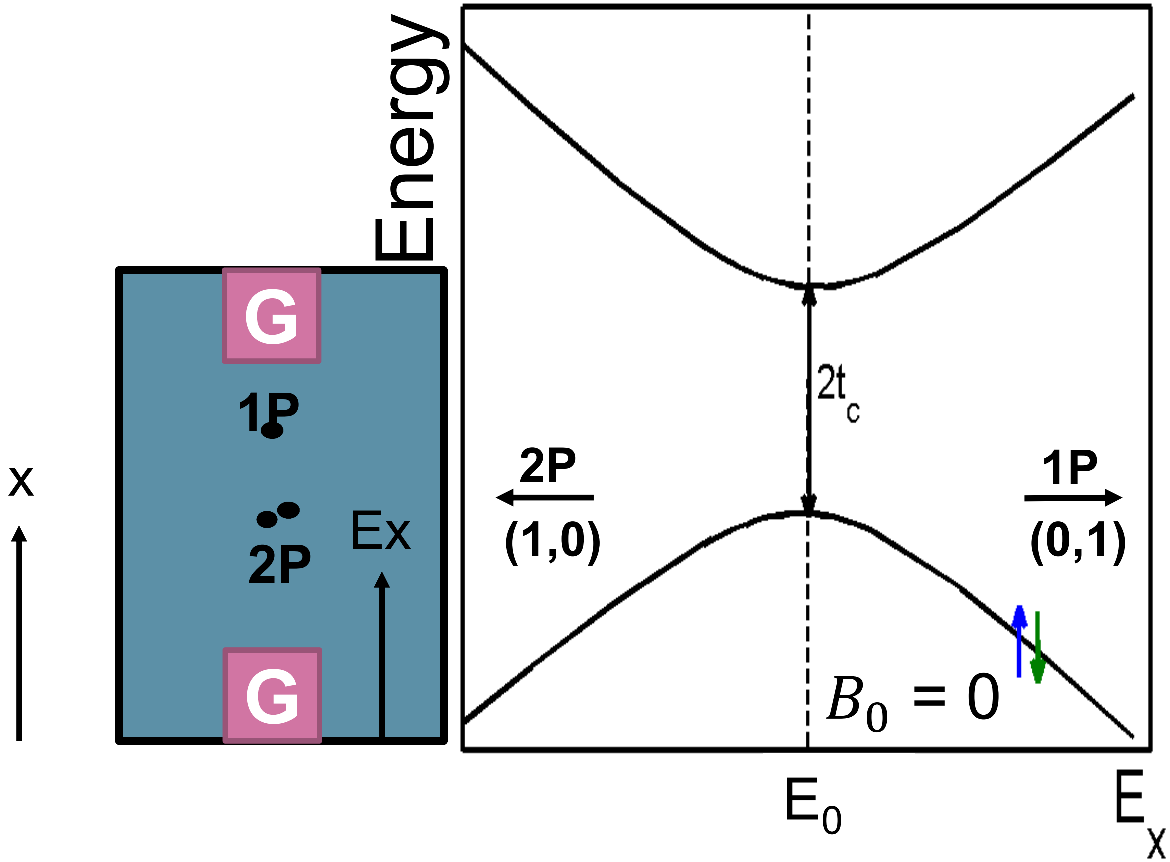
vs

$T_2^* = 11.61\ \mu s$



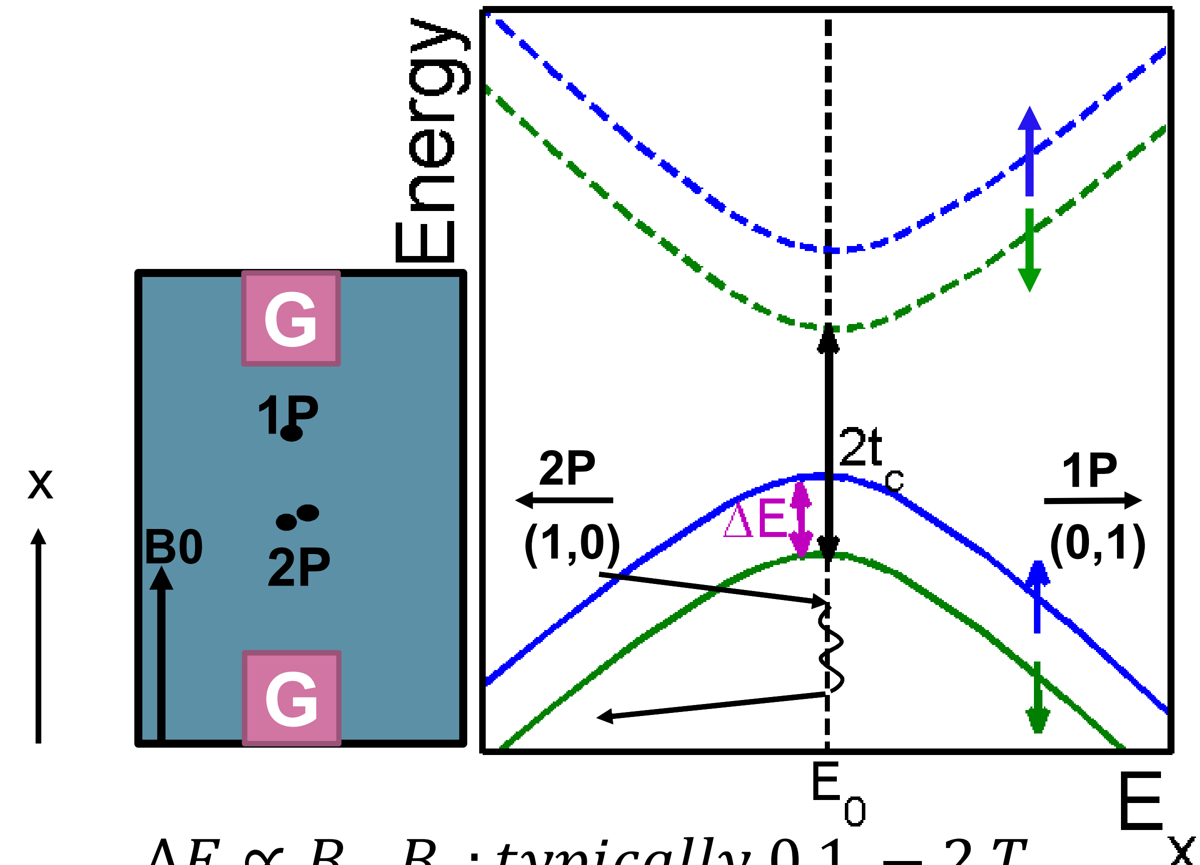
Consideration for control fidelity

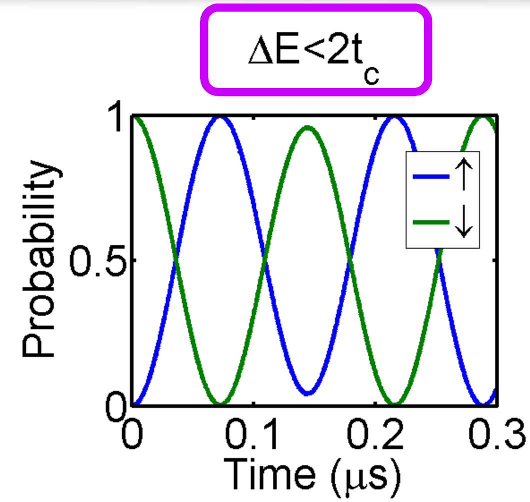
Charge energy diagram

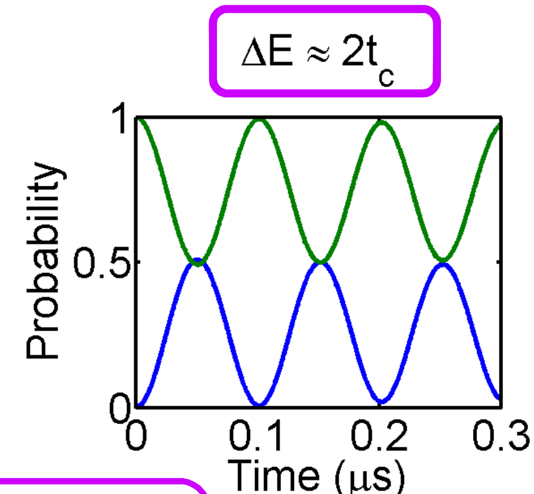


Consideration for control fidelity

Charge + spin energy diagram





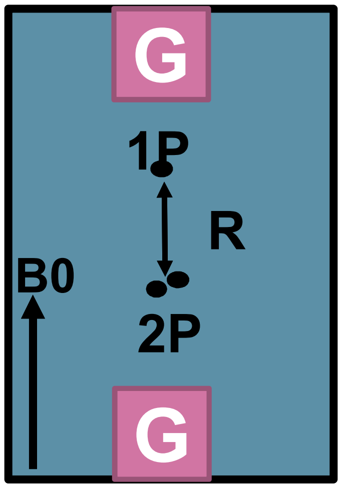


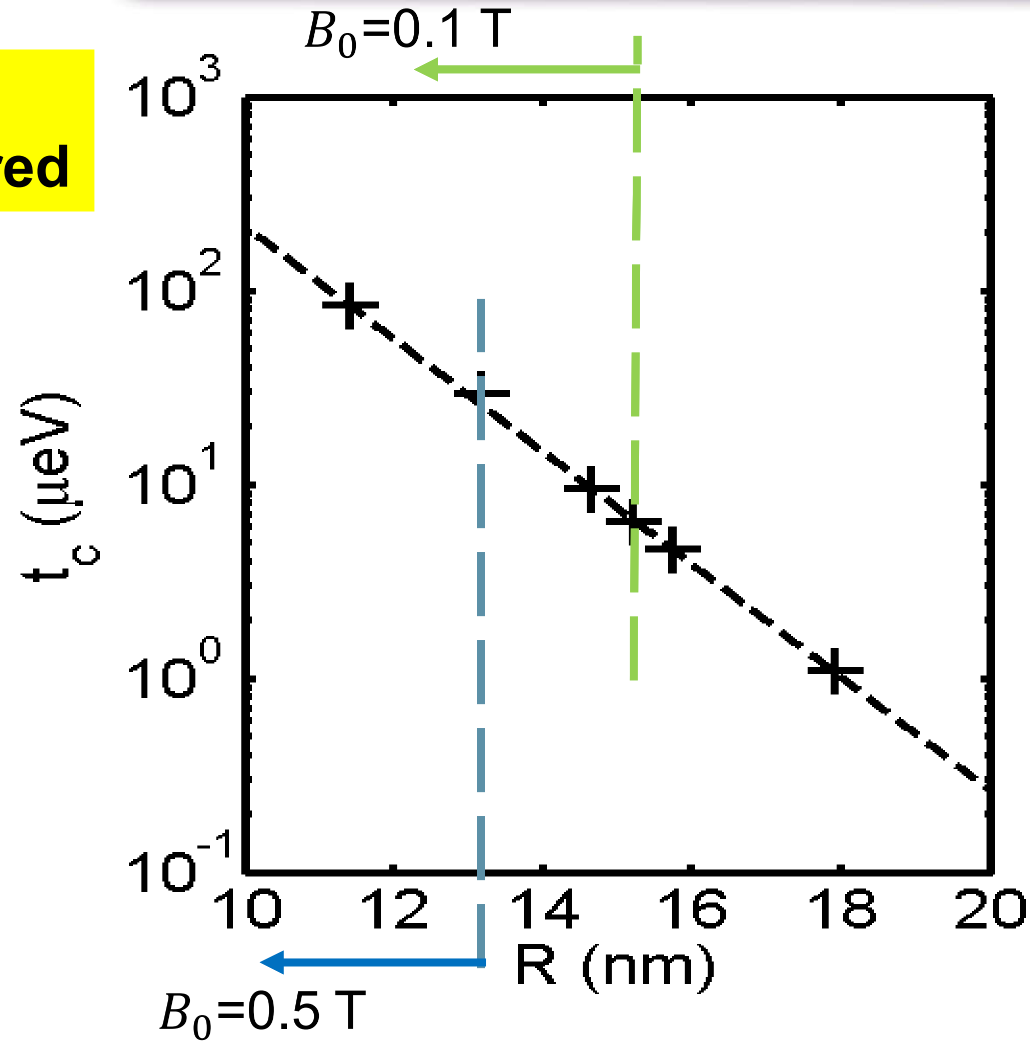
$\Delta E \propto B_0, B_0{:}\ typically\ 0.1 - 2\ T$

To achieve high control fidelity, $2\mathrm{t_c} > \Delta E$ is needed.
How to engineer t_c?

Choosing 2P-1P separation (t_c)

$\Delta E \propto B_0$,
$\Delta E < 2t_c$ **is required**





t_c decreases exponentially with R

To achieve high control fidelity, $R < 15\text{nm}$ is preferred.

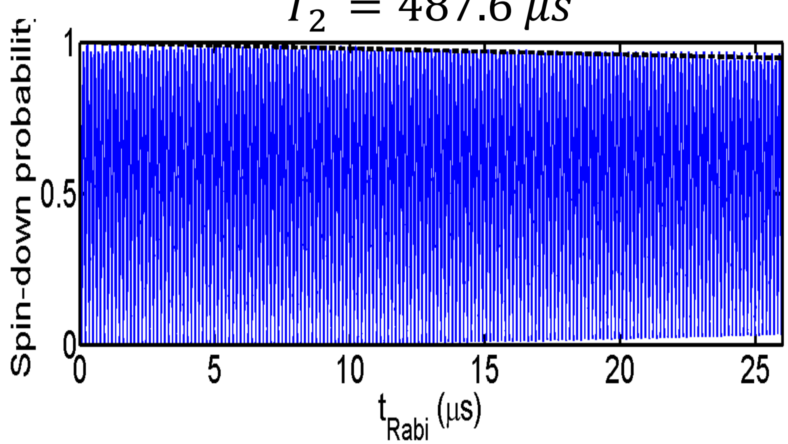
Coherence time

1. High control fidelity

3. Long spin storage time (no operation)

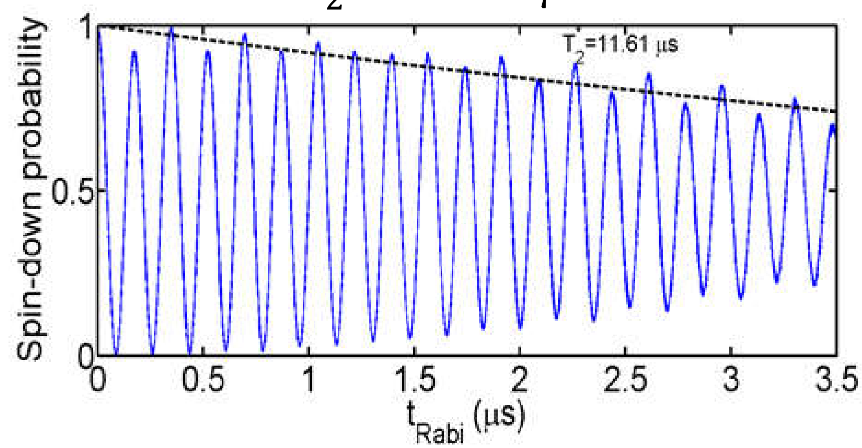
2. Long coherence time

$T_2^* = 487.6\ \mu s$



vs

$T_2^* = 11.61\ \mu s$



T_2^*: oscillation magnitude decays by e^{-1}

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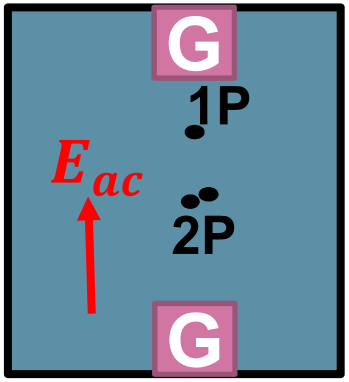
Coherence time calculation

Proposed method to calculate coherence time under charge noise

$$\frac{1}{T_2^*} = \frac{q^2}{\hbar^2} \left| \langle \Psi_\uparrow | r | \Psi_\uparrow \rangle - \langle \Psi_\downarrow | r | \Psi_\downarrow \rangle \right|^2 \left. \frac{S_E(\omega)}{\omega} \right|_{\omega \to 0} \frac{2 k_B T}{\hbar}$$

Chirolli & Burkard, Adv. in Phys., 57:3, 225-285 (2008).

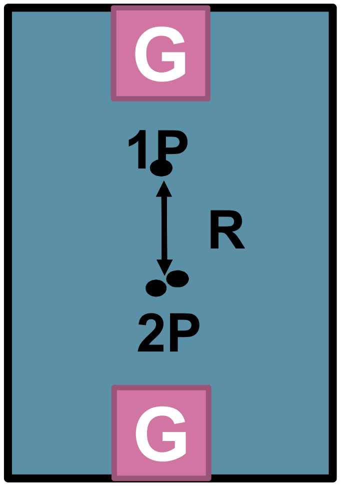


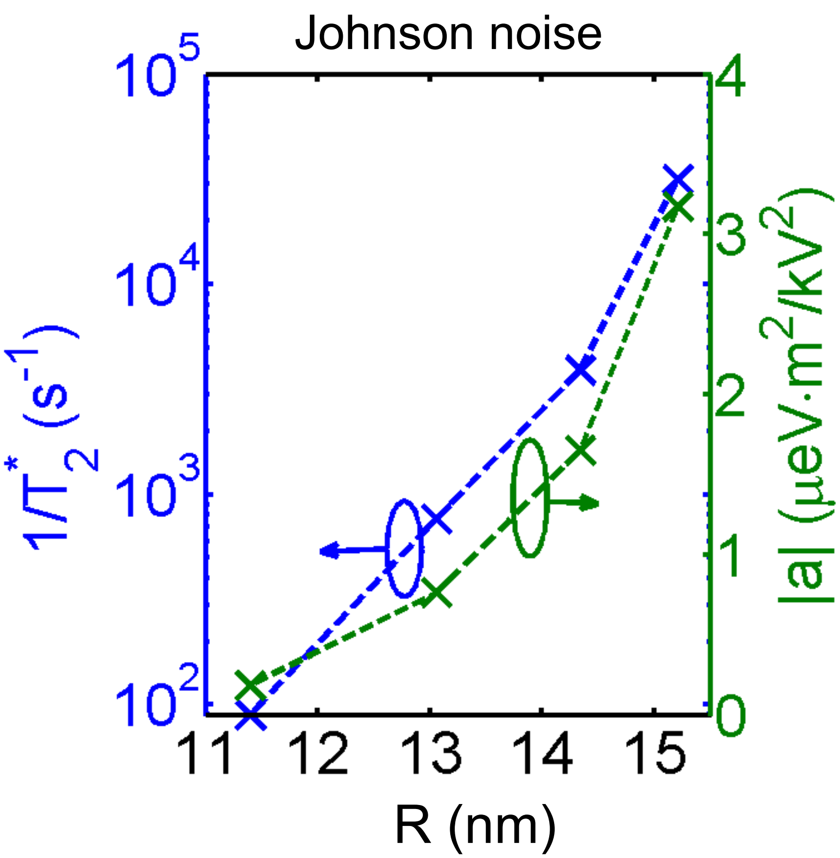
- Atomistic molecular wavefunction with electric-field, magnetic field and spin-orbit interactions.
- $S_E(\omega)$: Charge noise power spectrum
  1/f noise, Johnson noise, Evanescent wave Johnson noise

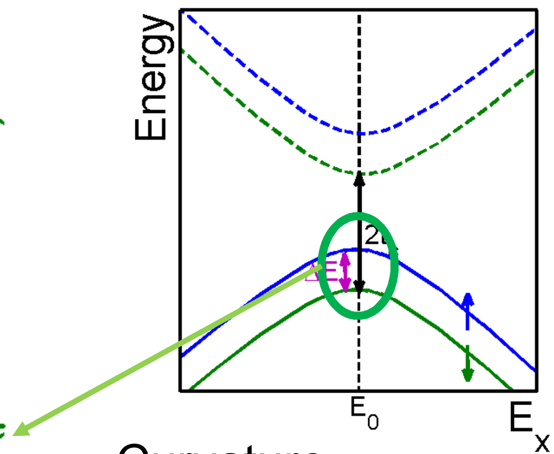
Noise spectrum Ref: P. Huang & X. Hu, PRB **89**, 195302 (2014)

Enabled decoherence calculation due to charge noise with an atomistic approach.

Impact of R on coherence time





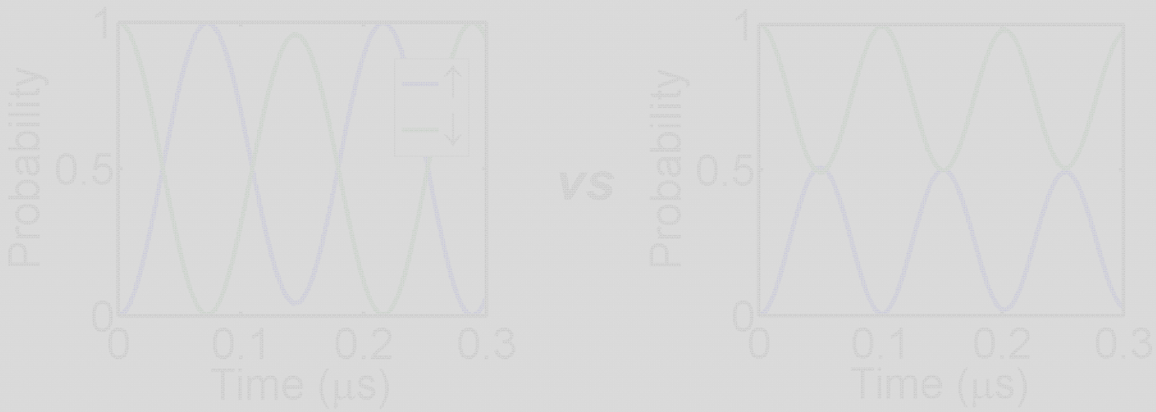


Curvature

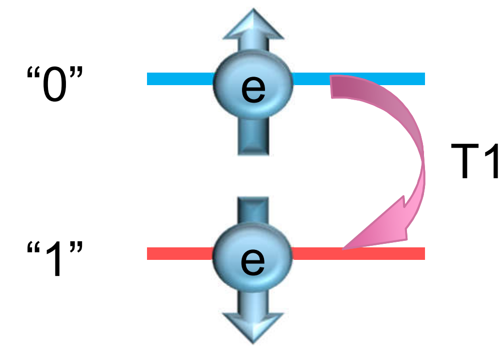
Larger curvature→ sharper charge transition→ more prone to noise

Smaller R is more favorable to suppress qubit decoherence due to charge noise.

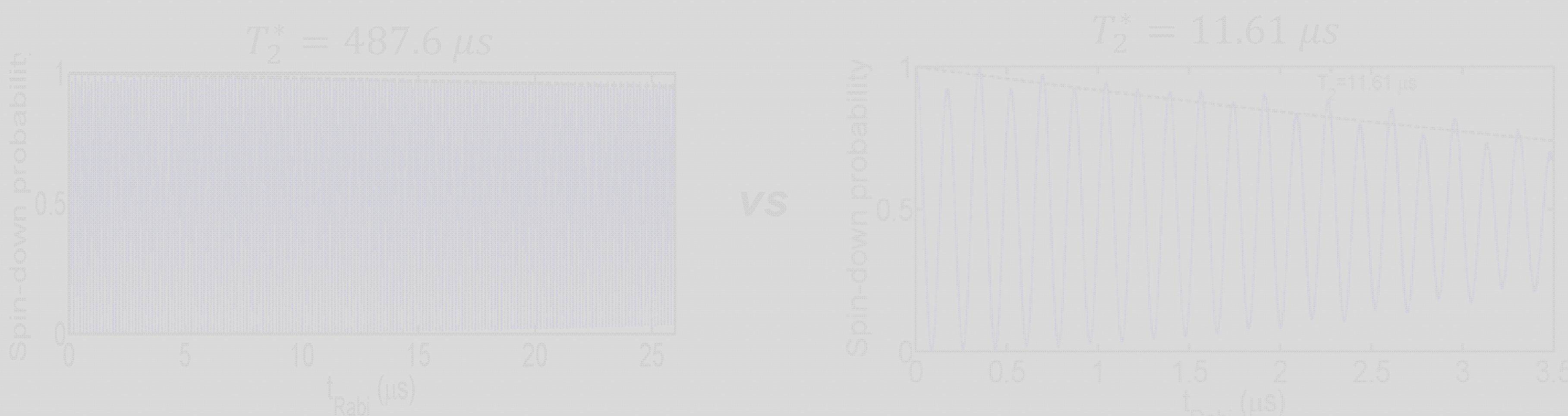
1. High control fidelity



3. Long spin storage time (no operation)

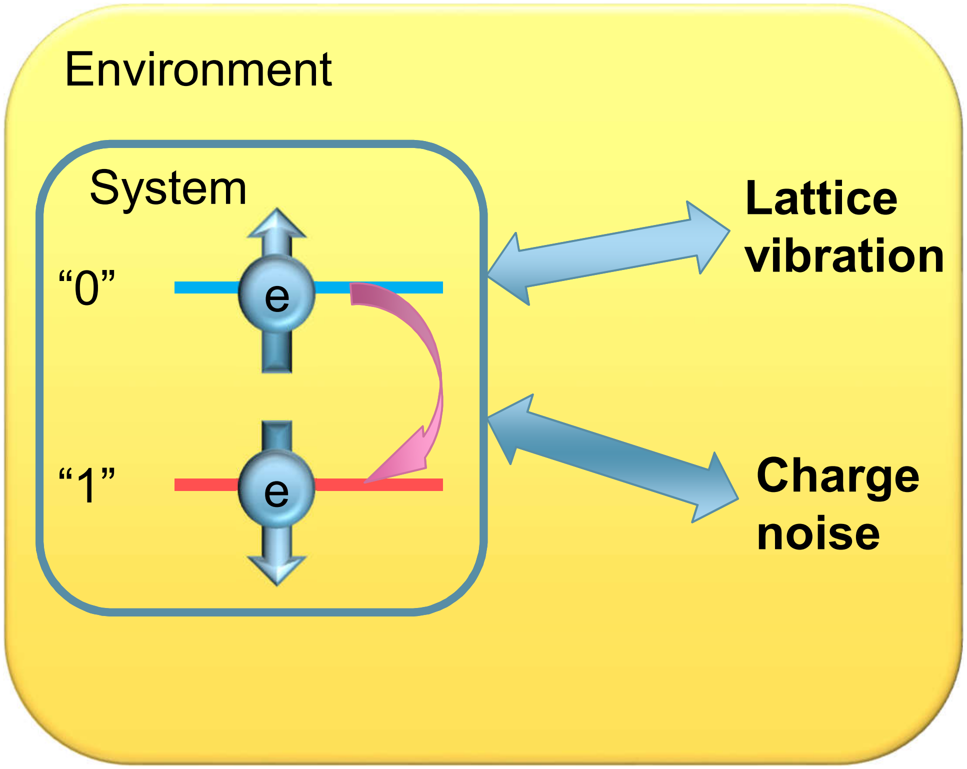


2. Long coherence time



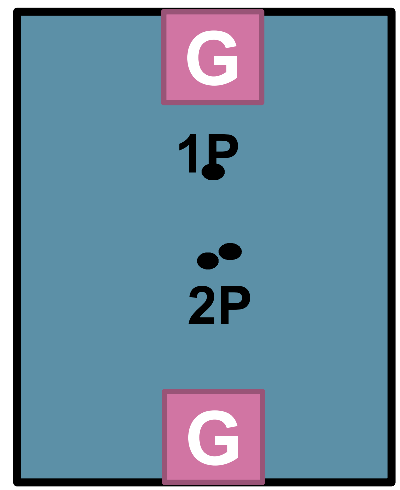
Future plan: investigate spin relaxation in the proposed design

Spin relaxation

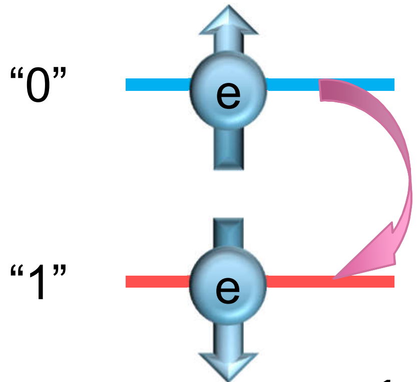


$$\mathbf{Pr}(\uparrow) \propto \mathbf{exp}\left(-\frac{\mathbf{1}}{\boldsymbol{T_1}}\right)$$

- Spin relaxation is critical for information storage (T_1 as long as possible)

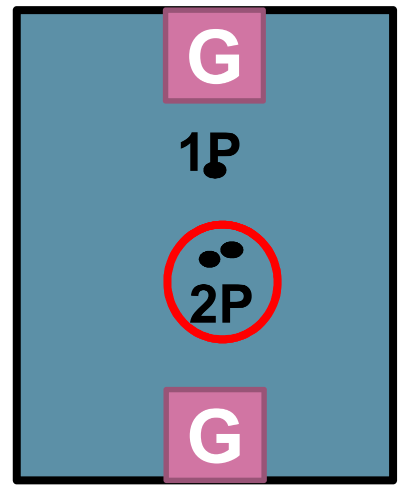


How to optimize T1 for information storage?



$$\Pr(\uparrow) \propto \exp\left(-\frac{1}{T_1}\right)$$

- Information storage: spin lifetime (T_1)
  - T_1(2P) ~= 30s, T_1(1P) ~= 4s.
    (Experiment: Watson et al., unpublished)

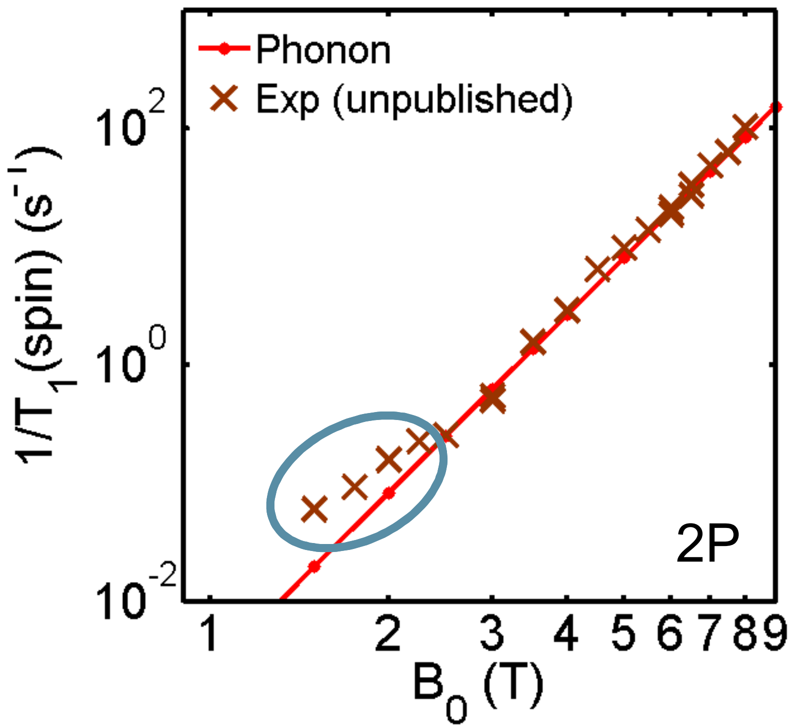


Qubit information is preferred to be stored in 2P.

What makes the spin relax?

- Mechanisms of spin relaxation:
  - Relaxation due to phonon

Hsueh et al., Phys. Rev. Lett. 113, 246406 (2014)



Exp. Data from T. Watson, unpublished.

Deviation at low B-field regime (<2.5T). Other mechanisms?

Mechanisms of spin relaxation: possibly charge noise

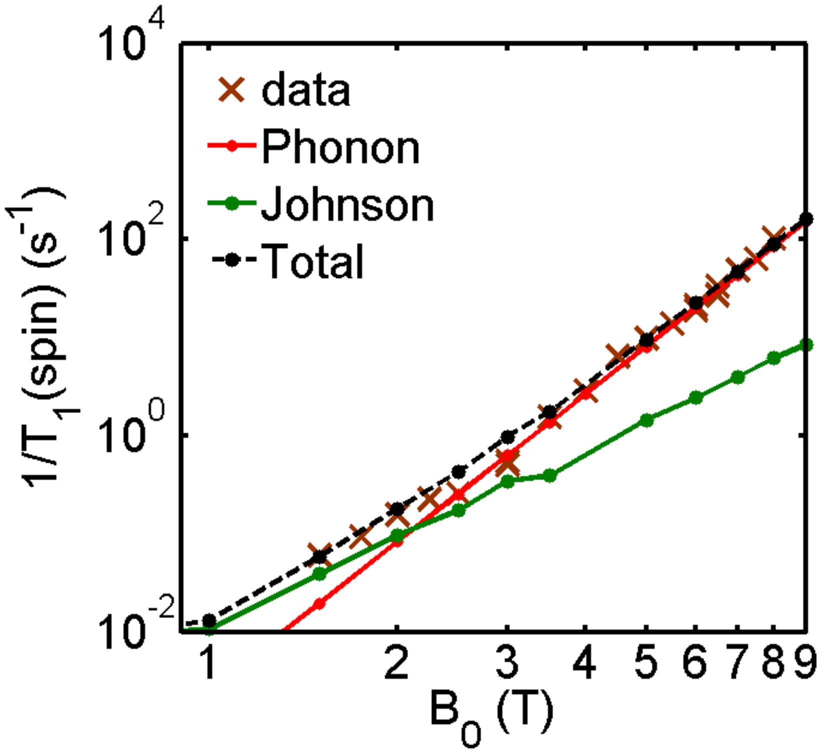
- Mechanisms of spin relaxation:
  - Relaxation due to phonon
  - Relaxation due to charge noise

- Developed formalism:

$$\frac{1}{T_1} = \frac{q^2 D D^*}{\hbar^2} S_E(\omega),$$

$$D = \sum_{o=x,y,z} \langle \Psi_\downarrow | o | \Psi_\uparrow \rangle$$

Deviation at low B-field regime is possibly due to charge noise.



Exp. Data from T. Watson, unpublished.

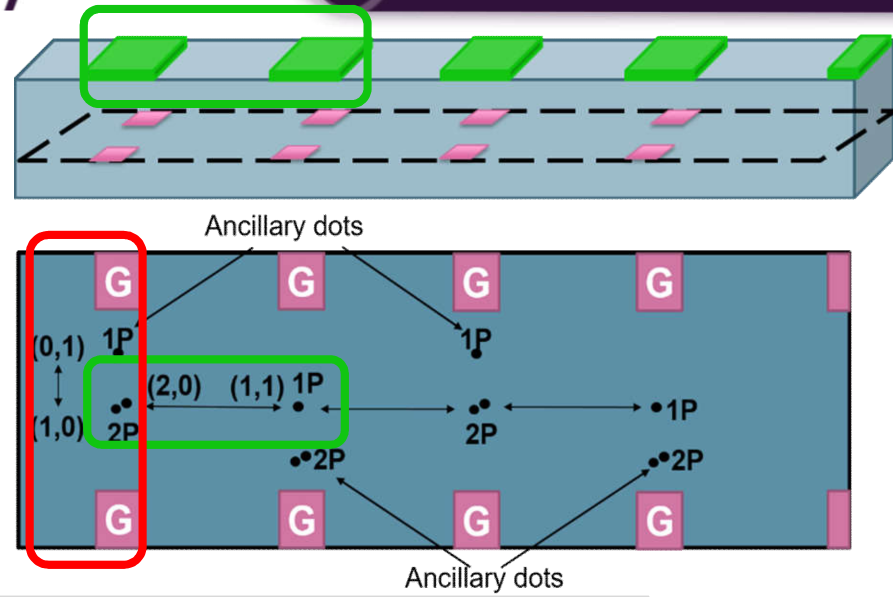
Summary of the 2P-1P qubit

To optimize electrical control of 2P-1P based spin qubit

1. **High control fidelity**
   -- optimization through R or tc (R< 15nm)

2. **Long coherence time**
   -- Johnson noise is the major influential factor
   -- optimization through R or tc (small R preferred)

3. **Long spin storage time (no operation)**
   -- 2P is preferred
   -- Johnson noise could be dominating over phonon in the low B-field regime



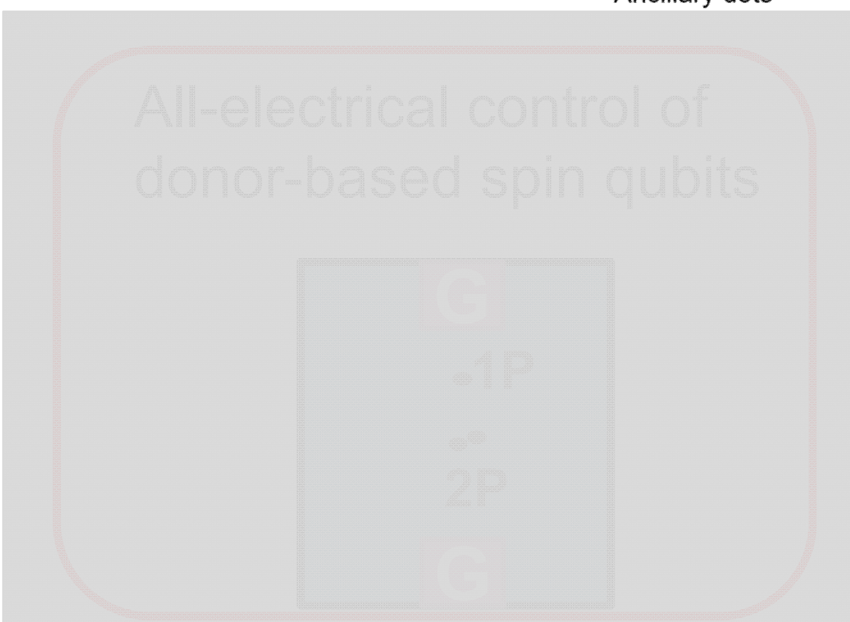
Overcome challenges in Kane's architecture

√ Fabrication:

  √ Gate separation

√ All-electrical control

√ Exchange tunability



Engineering exchange coupling of two donor qubits

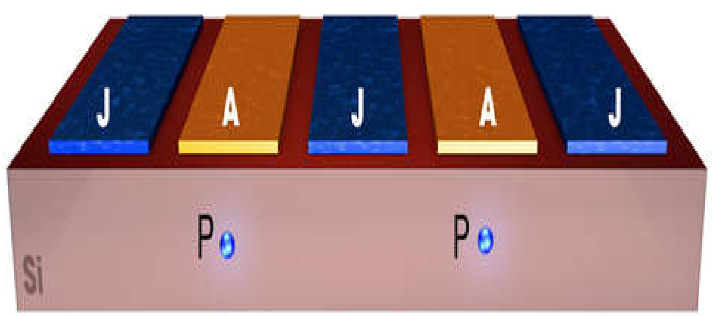
Challenges of Kane architecture

Challenges of realizing **multiple-qubit** operations using Kane architecture

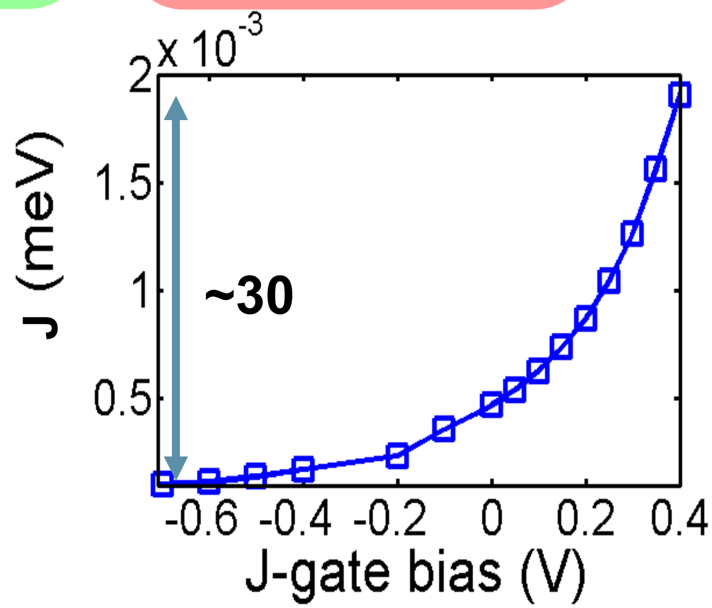
Fabrication

Magnetic control (single qubit)

Exchange control (2 qubits)



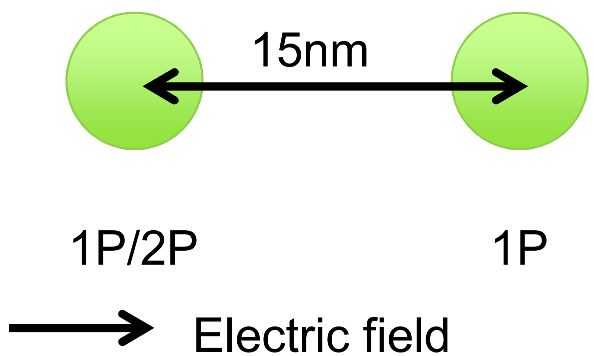
Kane, Nature 393, 133 (1998)



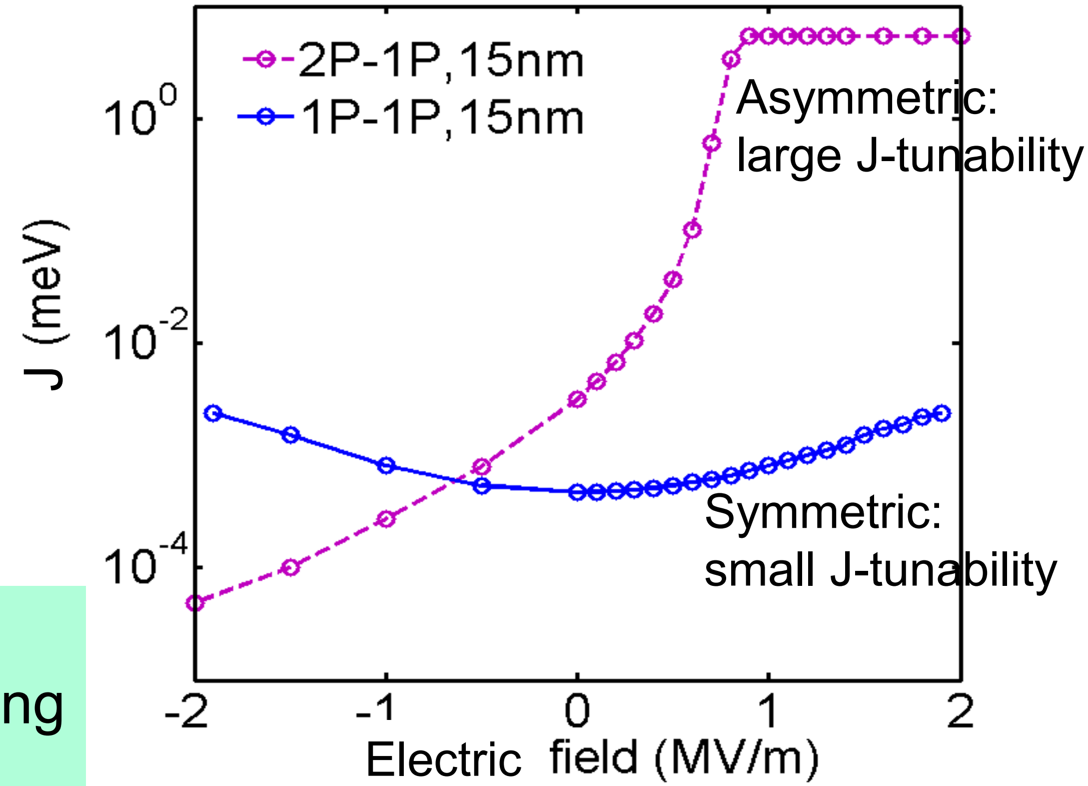
Does the 2P-1P system provide highly tunable exchange?

Symmetric vs asymmetric donor-based DQD: exchange tunability

J tunability with E-field



2P: the extra positive charge helps in attracting the 1P electron

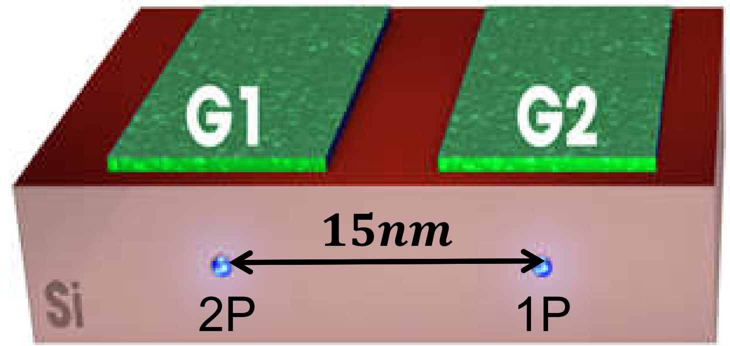


Over **5** orders of magnitude J tunability can be achieved within **3MV/m** detuning field (**48 neV** to **5.5 meV**).

Asymmetric 2P-1P systems are promising to realize two-qubit gates.

“Three is better than two”

- Using detuning gates is less challenging in fabrication.
- Exchange coupling can be tuned by over 5 orders of magnitude.



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ARTICLE OPEN

Highly tunable exchange in donor qubits in silicon

Yu Wang[1], Archana Tankasala[1], Lloyd CL Hollenberg[2], Gerhard Klimeck[1], Michelle Y Simmons[3] and Rajib Rahman[1]

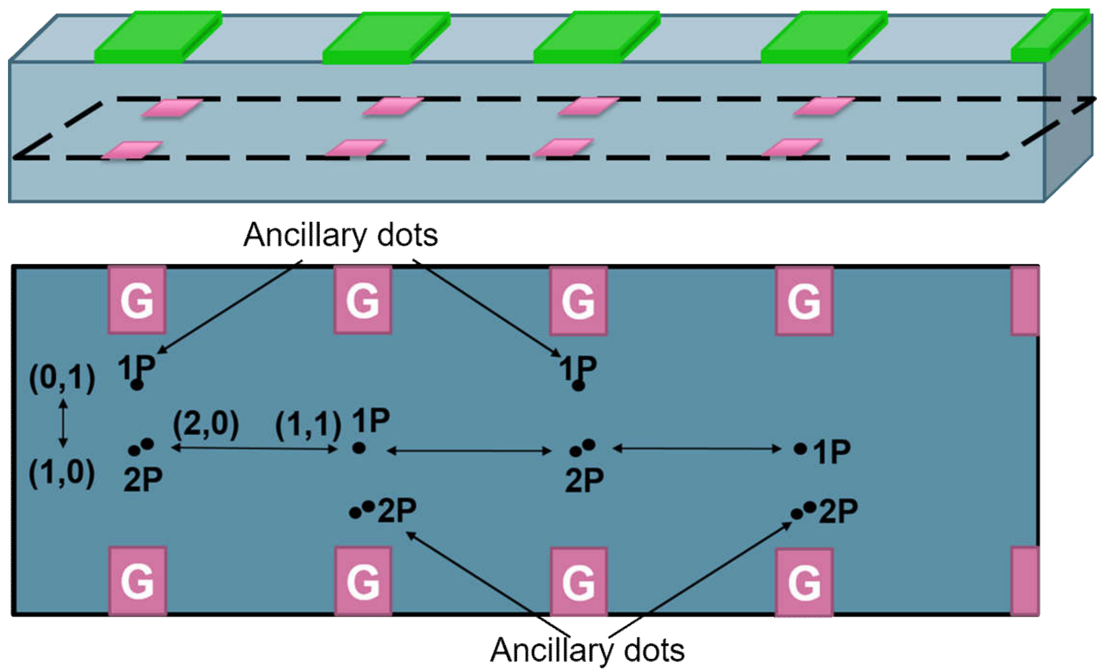
npj Quantum Information (2016) **2**, 16008; doi:10.1038/npjqi.2016.8; published online 12 April 2016

Summary of the proposed design

Lower Gate density

All-electrical control of spin qubits

High exchange tunability



A potentially scalable structure for donor-based spin qubits in silicon.

NEMO5

Acknowledgement

- Committee members:

  Professor Gerhard Klimeck, Dr. Rajib Rahman, Professor Supriyo Datta, Professor Zhihong Chen, Professor Michelle Simmons

- Archana Tankasala, Pengyu Long, Yuling Hsueh, Harshad Sahasrabudhe, Rifat Ferdous, Chin-Yi Chen, Yaohua Tan, Kai Miao, Hesameddin Ilatikhameneh, Fan Chen, Tarek Ameen, Yu He, Junzhe Geng, Prasad Sarangapani, Yuanchen Chu, Zhengping Jiang, Jun Huang, Xufeng Wang, Kuang-chong Wang and all my colleagues

- Professor Lloyd Hollenberg, Professor Andrew Dzurak, Holger Buch, Bent Weber, Thomas Watson, Matthew House, Sam Hile, Matthew Broome, Charles D. Hill, Menno Velderhost, Kok Wai Chan, Henry Yang, Wister Huang, Jianjun Zhang, Chunming Yin

- Ms. Vicki Johnson, Ms. Leslie Schumacher, Ms. Ashley Byrne

Thank you!

Backup

Other projects

- Characterizing Si:P quantum dot qubits with spin resonance techniques
  -- Wang et al., Sci. Rep. 6, 31830 (2016)
- Exchange engineering in MOS triple quantum dots
- Optimizing tunnel time for high-fidelity spin readout
- Electronic structure of donor bound exciton in silicon

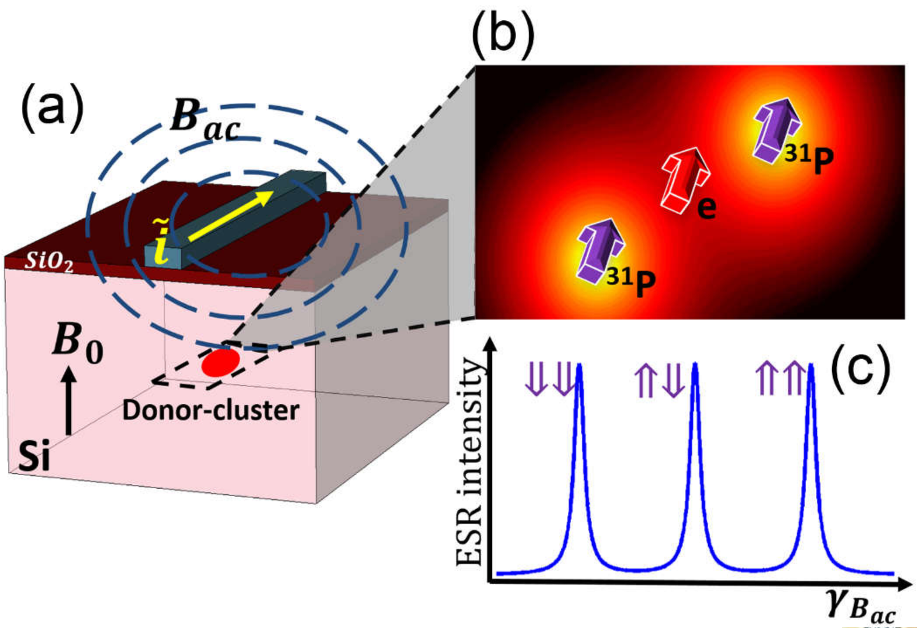
Characterizing Si:P quantum dots with spin resonance techniques (1)

Problem:
- There exists uncertainty in the configuration of a donor-cluster
- ESR of donor-cluster qubits hasn't been demonstrated experimentally

Objective:
- To characterize and manipulate donor-cluster spin qubits

Results / Impact:
- A non-invasive characterization technique
- More reliable and robust compared to the existing method based on measuring charging energies

Approach:
- Using electron spin resonance (ESR) techniques to measure ESR frequencies
- Map out the configuration of a donor-cluster by experiment-theory comparison



Y. Wang et al., submitted to Sci. Rep. (2016).

Characterizing Si:P quantum dots with spin resonance techniques (2)

NEMO5

Objective:

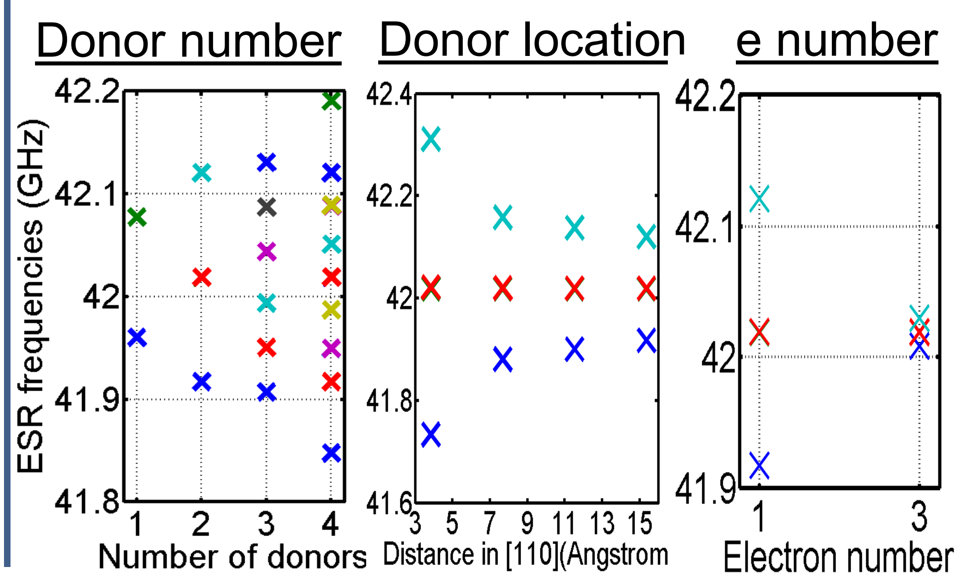
- To calculate the ESR spectra of donor-clusters with different donor numbers, locations and bound electron numbers

Results / Impact:

- Number of ESR frequencies goes up with number of donors.
- The separation of ESR frequencies decrease two-donor distance.
- The separations of ESR frequencies decrease with the bound electron number.

Approach:

- Obtain Fermi-contact hyperfine and dipolar interactions from atomistic tight-binding approach
- Obtain ESR spectra by solving effective spin Hamiltonian including Zeeman and hyperfine effects



Y. Wang et al., submitted to Sci. Rep. (2016).

Engineering exchange in MOS triple quantum dots (1)

Problem:

- To model a experimental device that has large active domain and multi-physics

Objective:

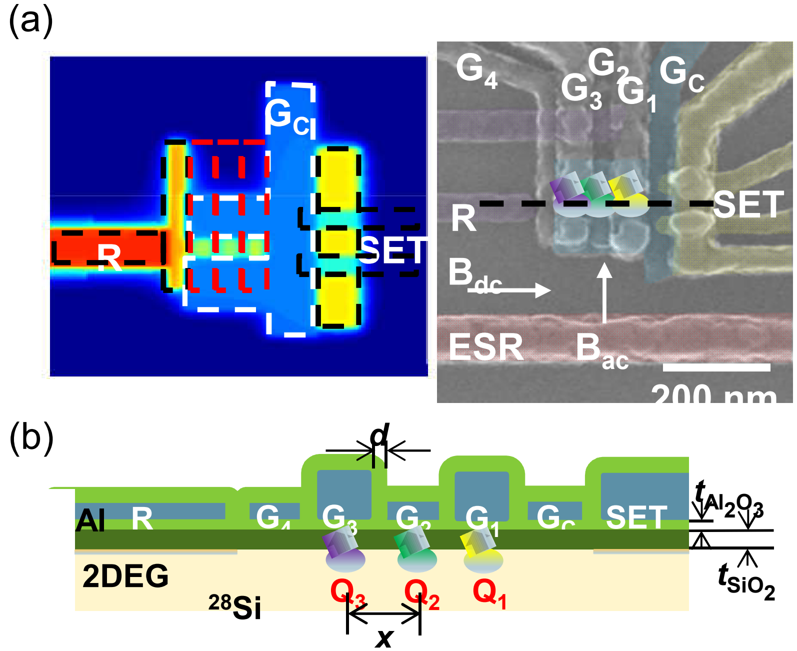
- To perform realistic simulations of electrostatics and electron wavefunction

Results / Impact:

- The multi-scale modeling scheme can handle simulations in the scale of μm
- Device physics like interface trap, work function difference, bandgap narrowing, incomplete ionization can be captured

Approach:

- Multi-scale modeling:
  - Semi-classical self-consistent charge/potential solution in the framework of TCAD
  - Quantum wavefunction solution with atomistic tight-binding approach



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Engineering exchange in MOS triple quantum dots (2)

Problem:

- To study the impact of device geometry on exchange energy

Objective:

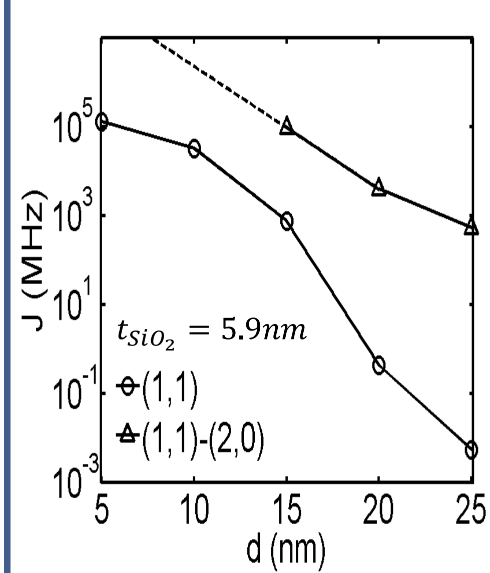
- To engineer and optimize exchange coupling in MOS quantum dot multi-qubit devices

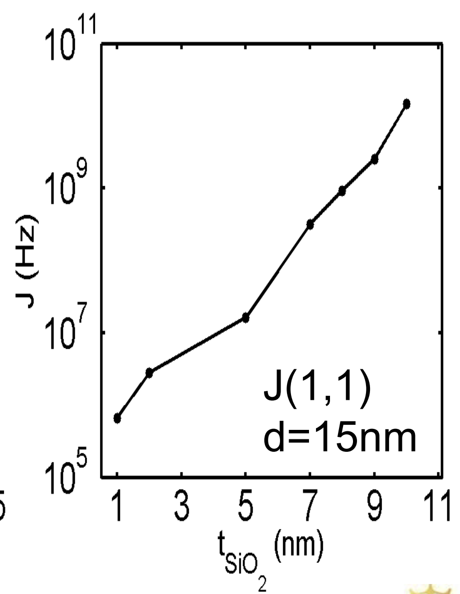
Results / Impact:

- The residue J ((1,1)) varies by ~7 orders of magnitude with d = 5-25nm; the active J((1,1)-(2,0)) is varied by ~2 orders of magnitude with d = 15-25nm; best match with experiment at d =23-24nm
- J((1,1)) varies by ~4 orders of magnitude with t_{SiO_2}

Approach:

- A full configuration interaction (FCI) method for electron-electron exchange calculation, which accurately captures exchange and correlations, with the atomistic tight-binding basis.





Optical readout with donor bond exciton

Problem:

- Optical readout haven't been utilized in single donor spin qubits.

Objective:

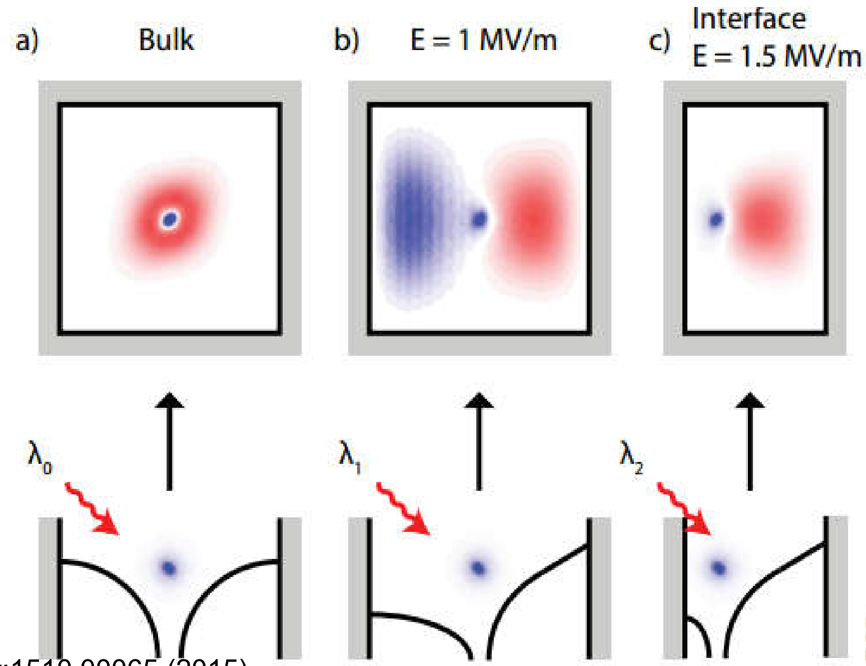
- To investigate the electronic structure of D^0X in silicon under the influence of electric fields and interfaces.

Results / Impact:

- The calculated bulk transition energy (1145meV) is close to the reported experimental measurements (~1150meV)
- Provide quantitative guidance to experiments aiming to realize hybrid opto-electric techniques for addressing donor qubits

Approach:

- Atomistic tight-binding approach for electron and hole wavefunctions
- Developed Hartree self-consistent field method for three-particle (2e+1h) quantum solutions



R. Rahman et al. arXiv:1510.00065 (2015).

Optimizing tunnel time for high-fidelity spin readout (1)

Problem:

- A comprehensive quantitative theory that can provide design guidance for spin readout devices using a quantum mechanical description is lacking.

Objective:

- To interpret the tunnel time of experiment qubit devices.

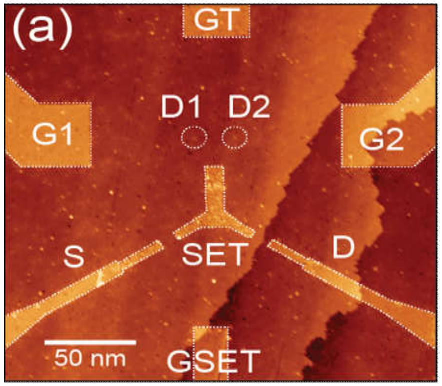
Results / Impact:

- Proposed a comprehensive theory based on atomistic modeling for tunneling time calculation in spin readout devices.
- Bandgap narrowing effect can be captured

Approach:

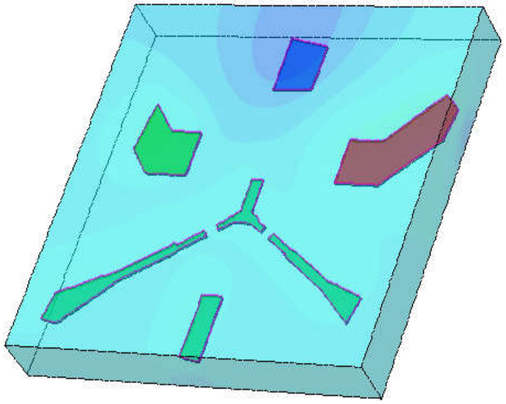
- Multi-scale modeling:
    - Semi-classical approach for the electrostatic solution of the SET island in the framework of Sentaurus TCAD tool.
    - Atomistic tight-binding for donor and SET wavefucntion

Experiment



T. Watson et al., Phys. Rev. Lett. 115, 166806 (2015)

TCAD modeling



Optimizing tunnel time for high-fidelity spin readout (2)

Problem:

- To optimize the tunnel time for single-shot readout to achieve high-fidelity

Objective:

- Provide guidelines for SET-donor separation to achieve high-fidelity spin readout

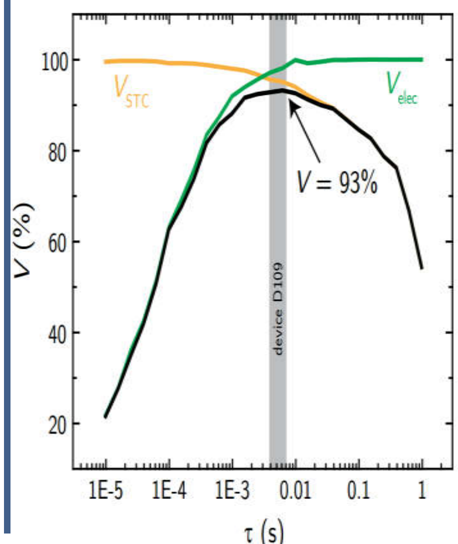
Results / Impact:

- Proposed a comprehensive theory based on atomistic modeling for tunnel time calculations
- The tunneling time between the qubit and the SET island can vary by ~5 orders of magnitude with their separation changing by ~10 nm, and is sensitive to the qubit net charge

Approach:

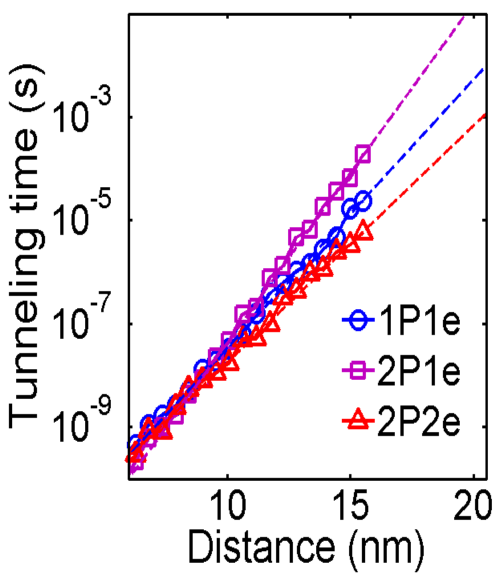
- Utilize the impurity model in the frame work of atomistic tight-biding approach
- Hartree self-consistent field approach to capture multi-electron occupation
- Use Bardeen's tunneling theory to calculate tunnel time

Fidelity vs tunnel time



H. Buch, Ph.D. thesis (2014).

Calculation



A two-qubit logic gate with donor-based qubits

Problem:

- Two-qubit logic haven't been demonstrated with donor-based spin qubits

Objective:

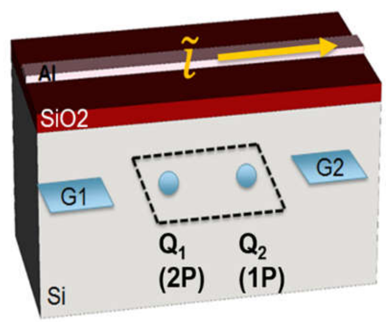
- To provide guideline for realizing a CNOT gate with donor-based qubits experimentally

Results / Impact:

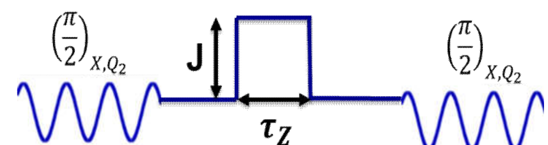
- Theoretical evidence that a CNOT gate is feasible with donor-based qubits
- Provide guidelines to optimization for experiments.

Approach:

- Use ESR to address individual spin qubits.
- Use detuning bias to control the exchange coupling between the two qubits
- Modeling: atomistic tight-binding + configuration interaction + effective spin Hamiltonian



- CNOT is realized with J=~26GHz and τ_Z = ~294.77 ns



Veldhorst et al., Nature 526, 410–414 (2015)