

Electron Spin Relaxation of Donors in Silicon Nanoelectronic Devices

FINAL EXAMINATION

PURDUE
UNIVERSITY

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Introduction to quantum computing and T_1

The spin-relaxation mechanisms : Existing theories

Part I: The tight-binding T_1 method

Part II: T_1 in device with electric fields

Part III: Two-electron T_1 problem

Introduction to quantum computing and T_1

The spin-relaxation mechanisms : Existing theories

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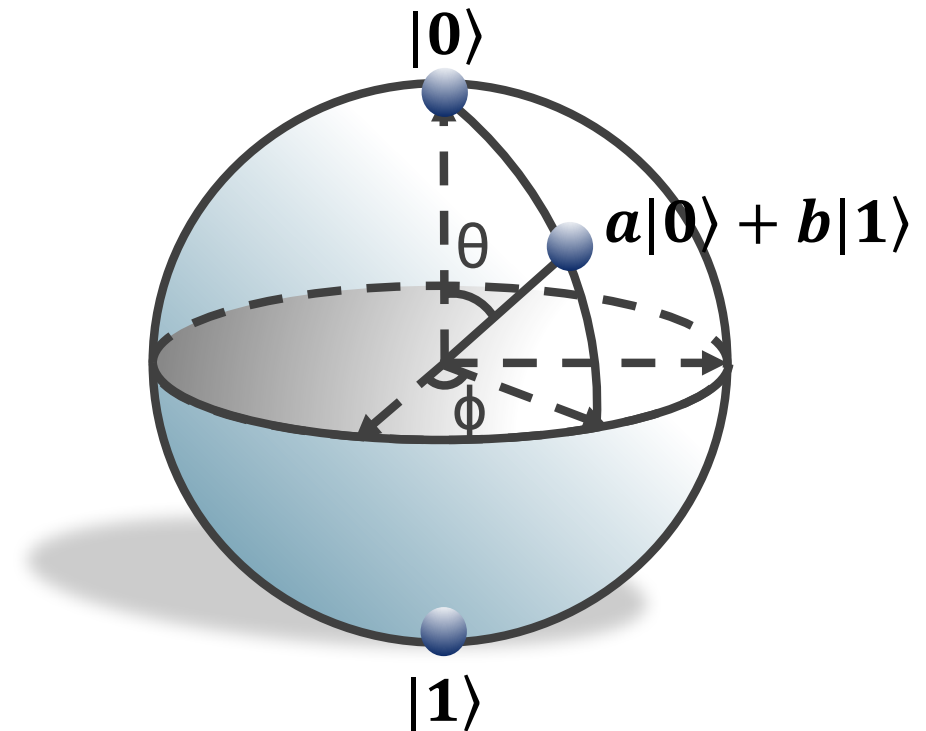
A Single Qubit

— $|0\rangle$
— $|1\rangle$

Qubits:

- Two basis states $|0\rangle$ and $|1\rangle$
- Superposition $a|0\rangle + b|1\rangle$

The Bloch Sphere

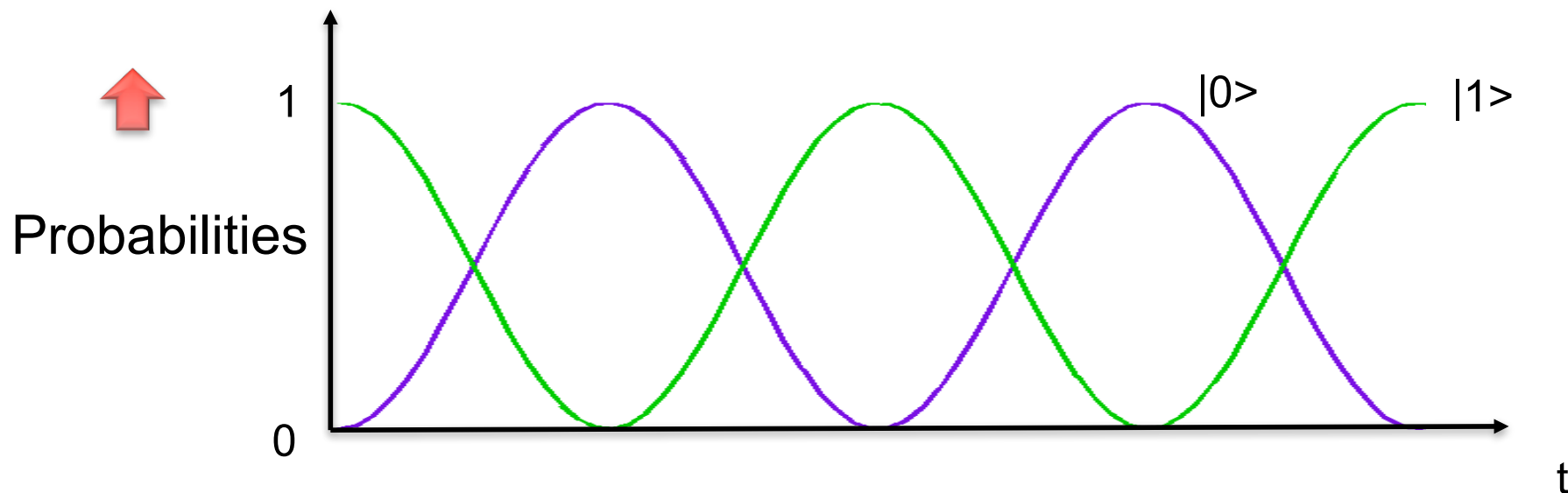
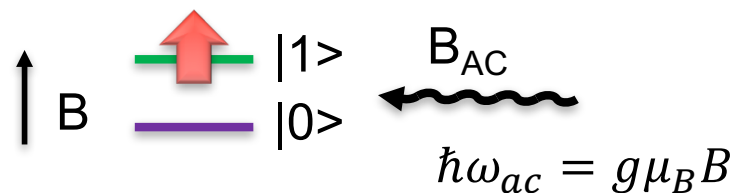


Classical bits: $|0\rangle, |1\rangle$

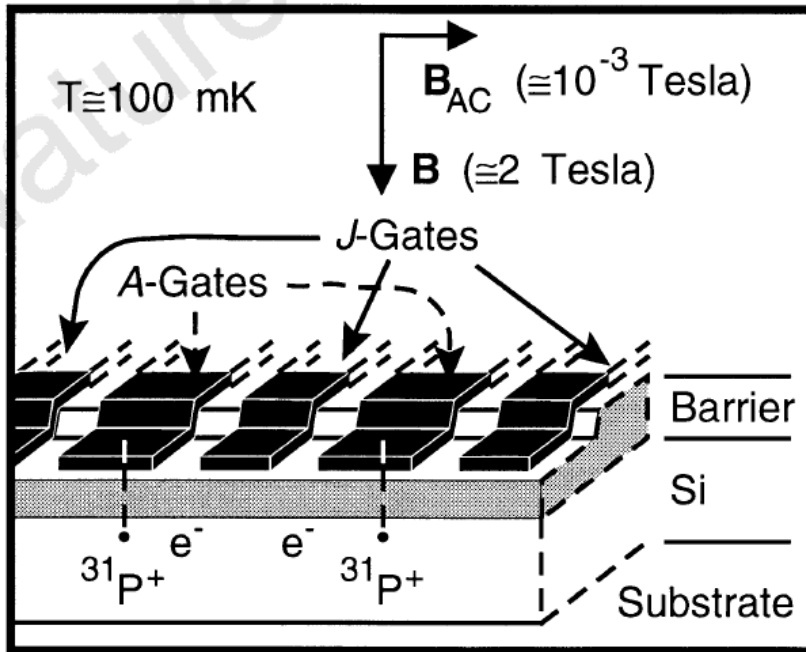
Qubits: $|0\rangle, |1\rangle, 0.71|0\rangle + 0.71|1\rangle, 0.71|0\rangle - 0.71|1\rangle, \dots$

B field \rightarrow split spin states

$B_{AC} \rightarrow$ rotate the spin

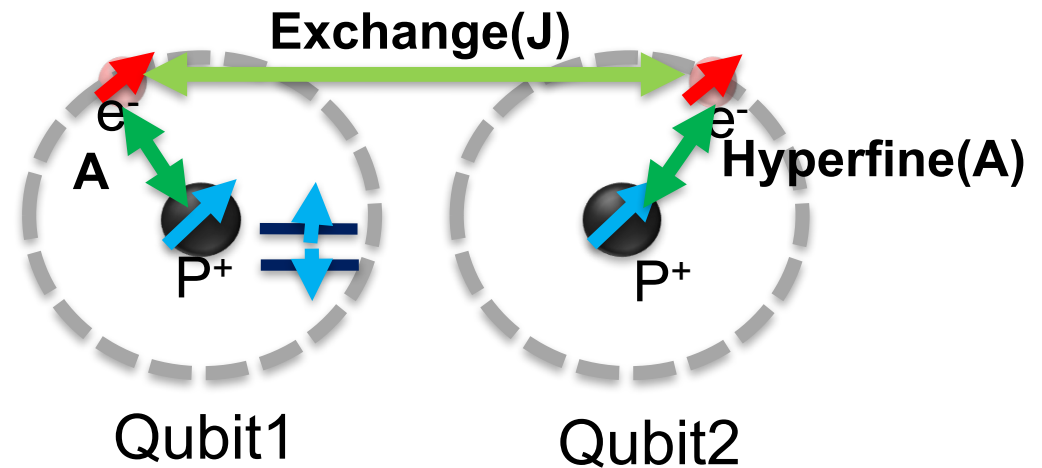


Qubit operation: time evolution of two coherent states.



Kane, Nature 393, 133 (1998)

Kane's Architecture

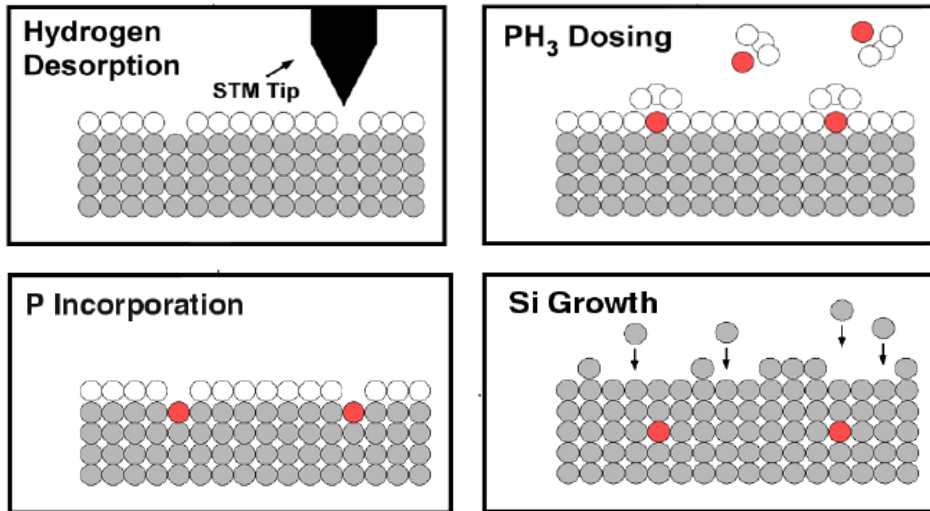


Si donor spin qubit:

- encodes information in the nuclear spin
- 1 donor confines 1 electron
- electron wf can be tuned by gates
→ changes resonance frequencies

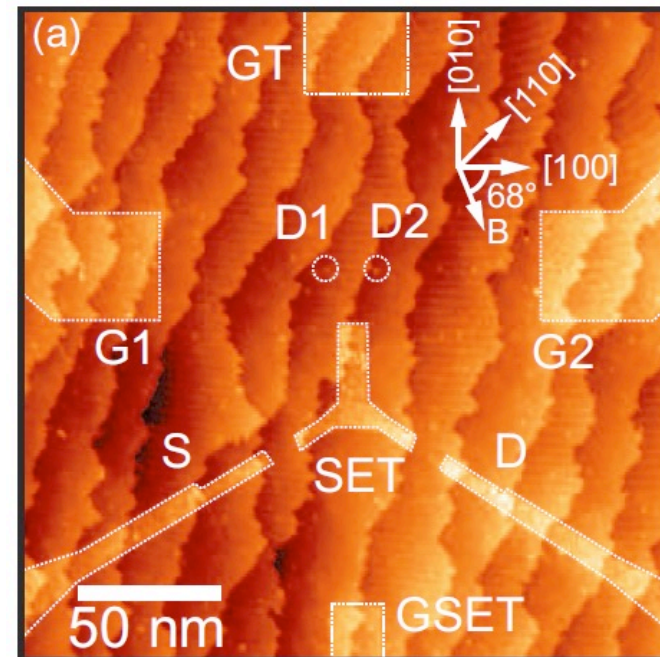
Kane proposed using donors in Si nano-devices to build a quantum computer.

Scanning Tunneling Microscope (STM)



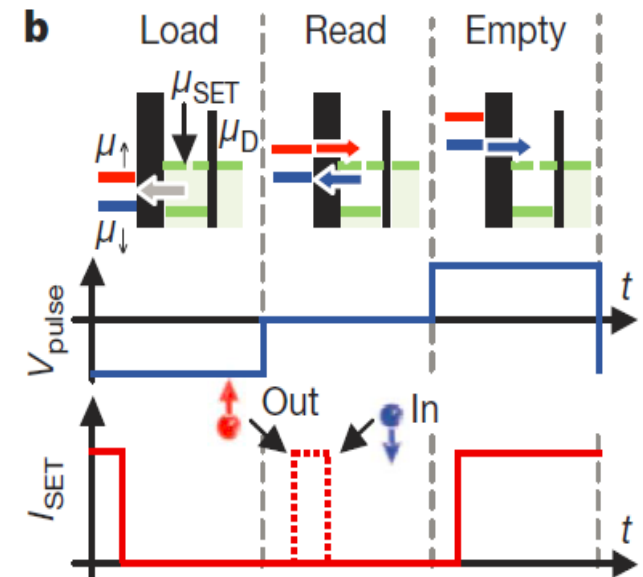
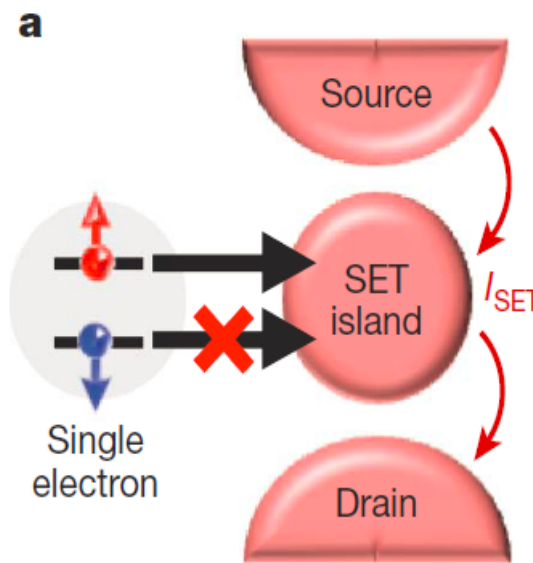
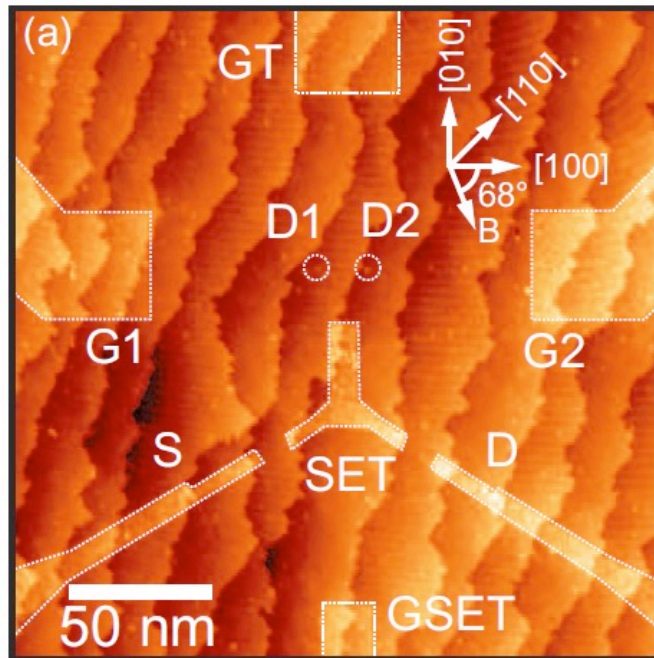
“2013_SISC_Tutorial” by Michelle Simmons

- Put a single P atom in a specific location.
- Construct 2D delta-doped P in Si gates.



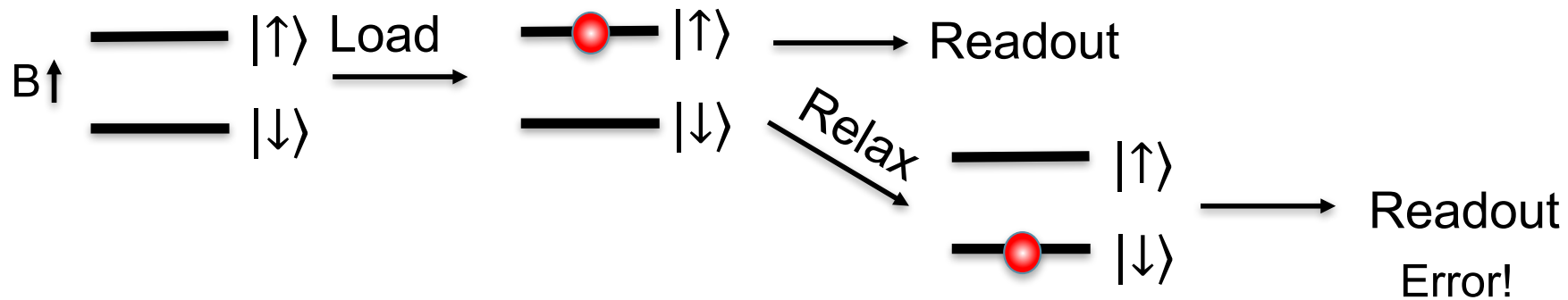
Single-atom STM
fabricated device

STM technique → realize Kane's architecture.



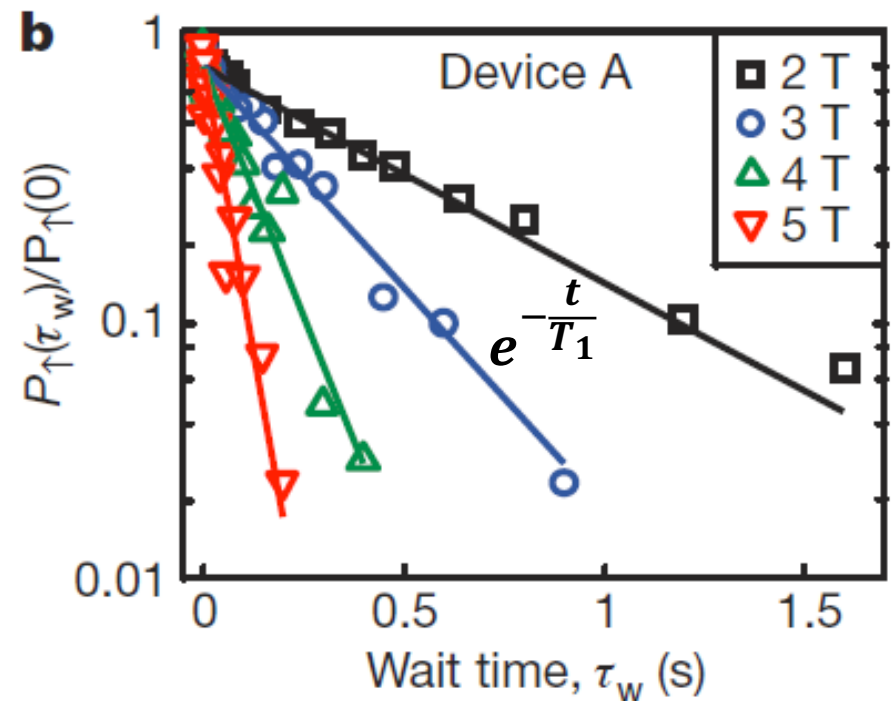
- Change gate voltages such that the donor's electron can tunnel to/from the SET and change the source to drain current.

Tunnel to a nearby SET → load/read the electron



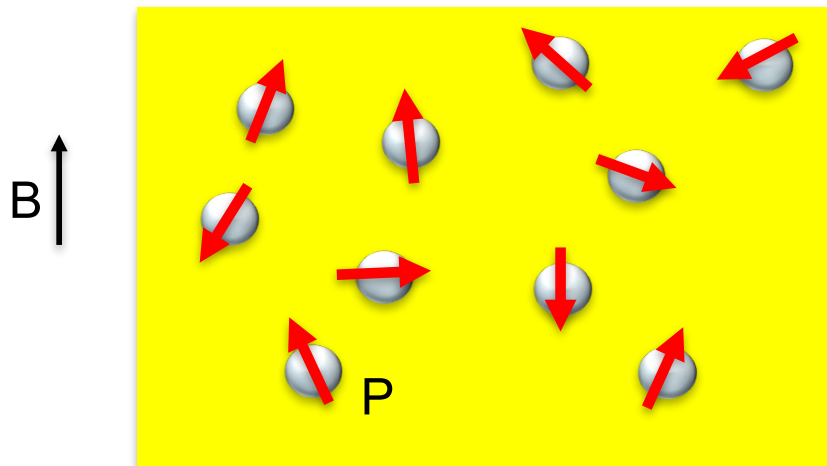
- Long $T_1 \rightarrow$ High fidelity
- Represents coupling to the environment.
- Serve as an upper bound to T_2 .

Long T_1 is desirable.



T. F. Watson et al., Science Advance, DOI: 10.1126/sciadv.1602811 (2017)

A. Morello et al. Nature 467, 687 (2010) 9

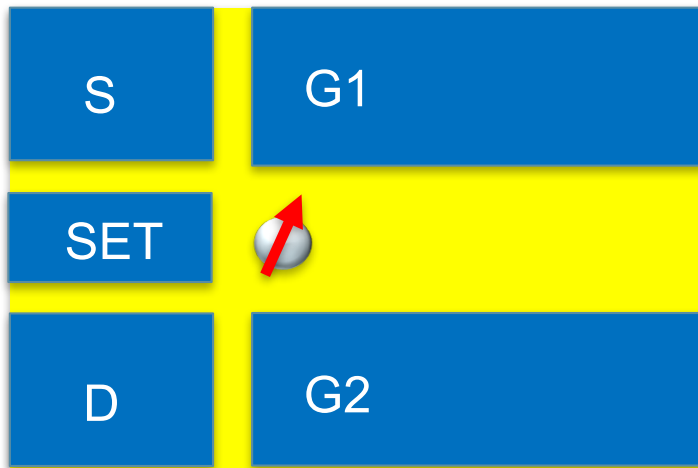


Donors in bulk Si

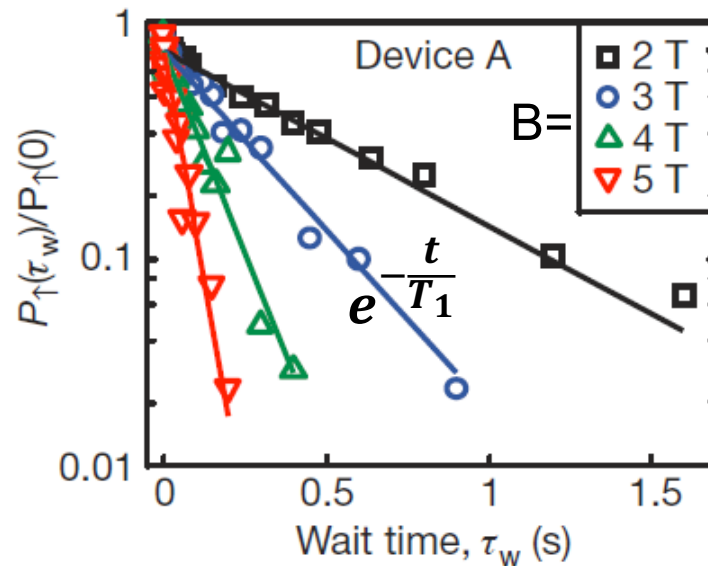
Magnetization M of the whole sample

$$M = M_0(1 - e^{-\frac{t}{T_1}})$$

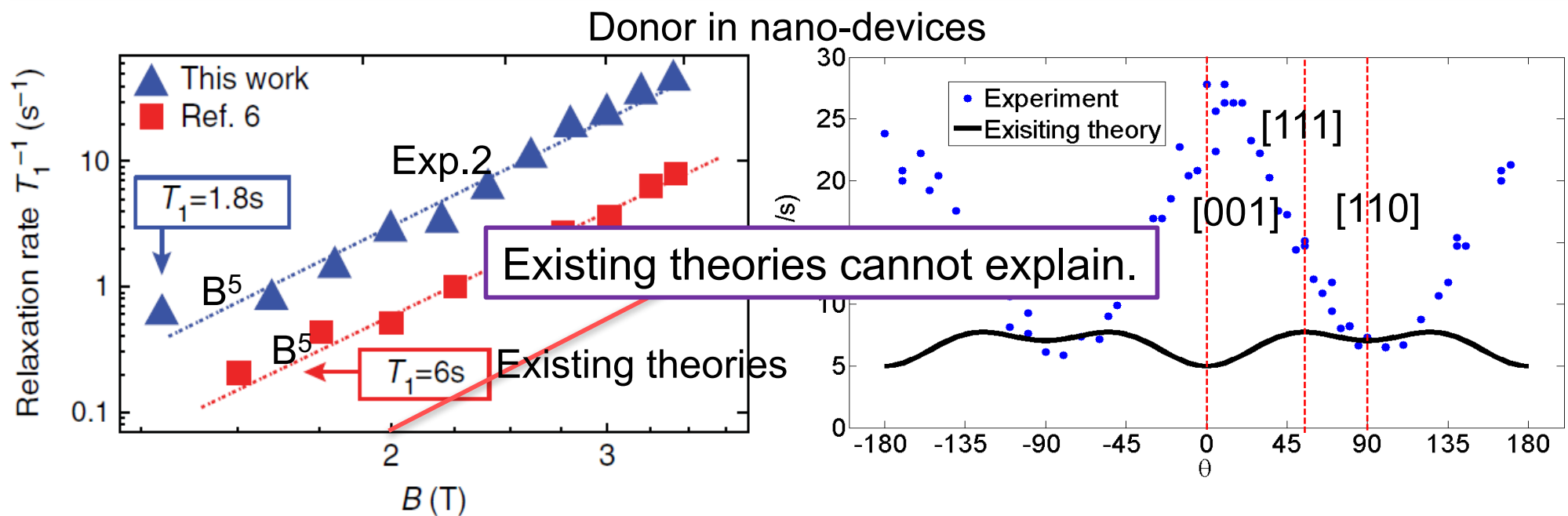
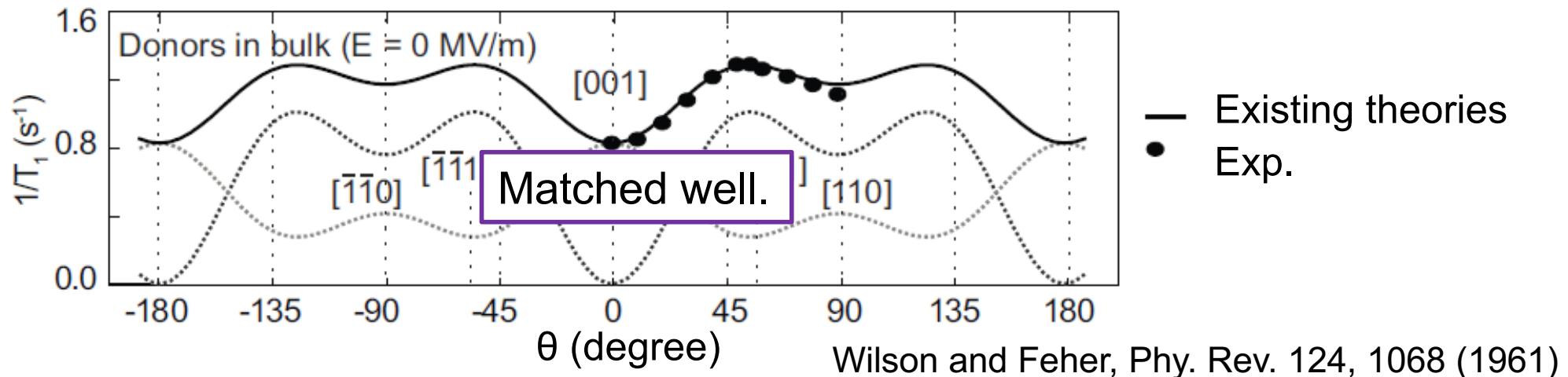
Local environment doesn't matter.



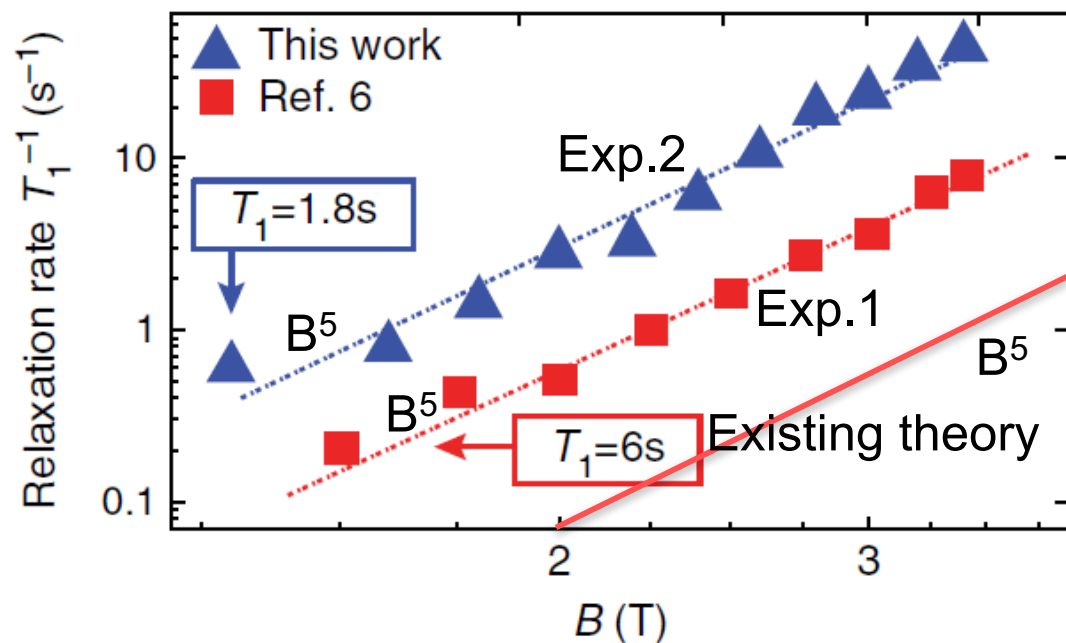
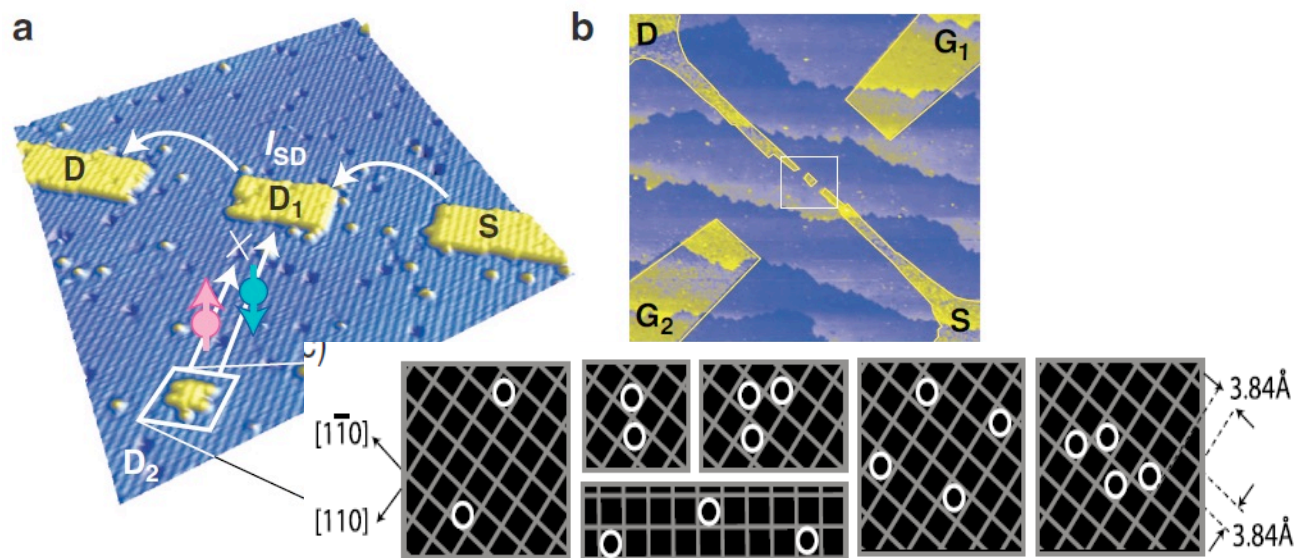
Donor in nano-devices



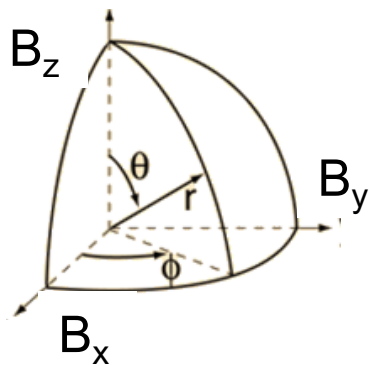
Local environment becomes very important.



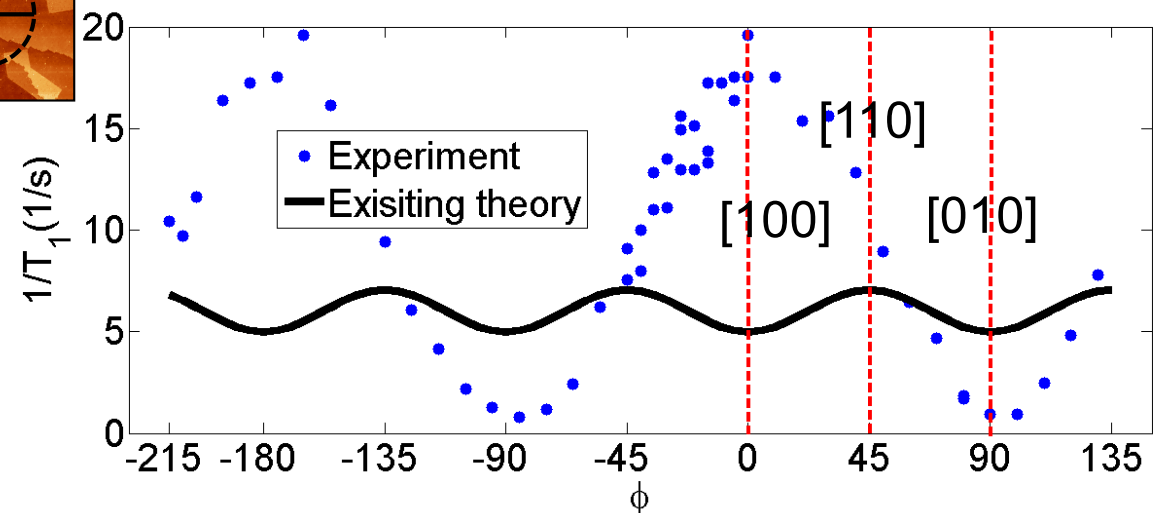
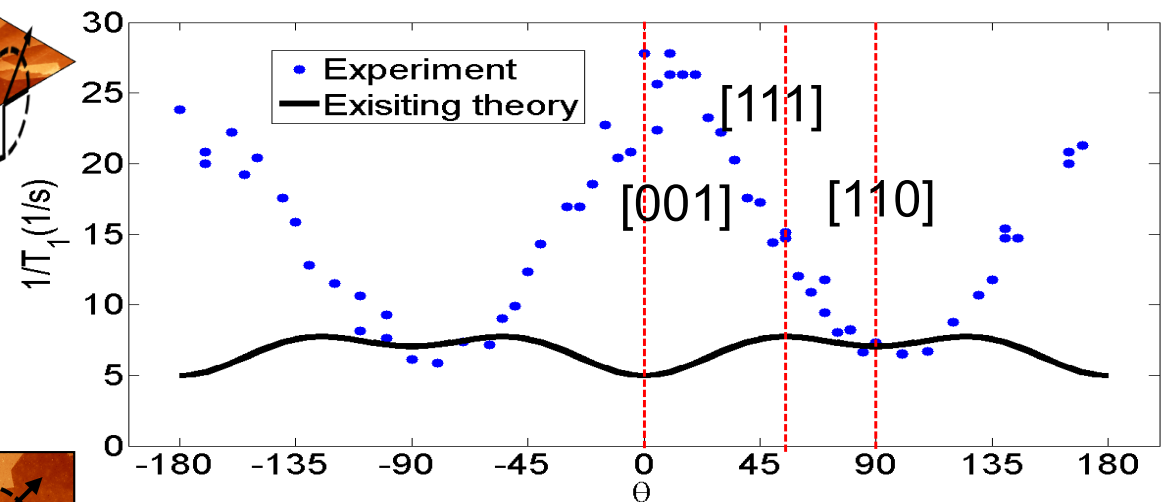
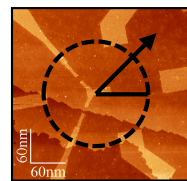
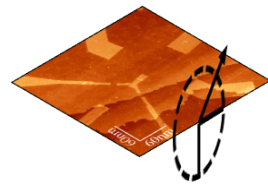
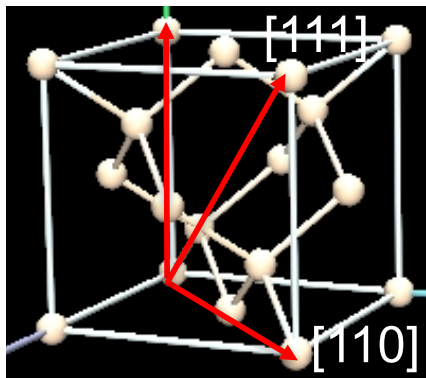
B. Weber et. al., "A Single-Atom Probe of the Silicon Qubit Environment" (submitted) H. Büch et al. Nature Communications 4, 2017 (2013)



Problem: Existing theories only consider single donors.
 → Need a comprehensive approach to calculate T_1 in donors and donor clusters.

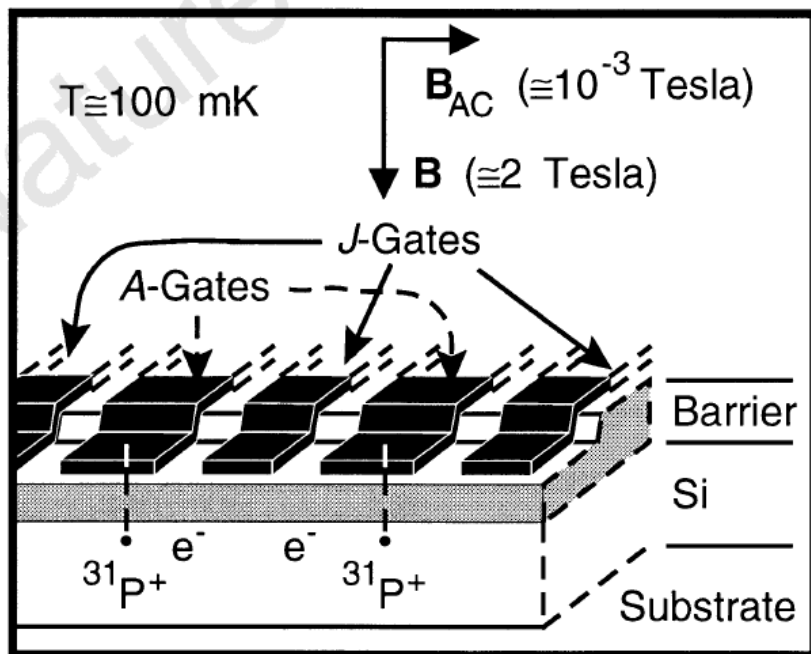


[001]



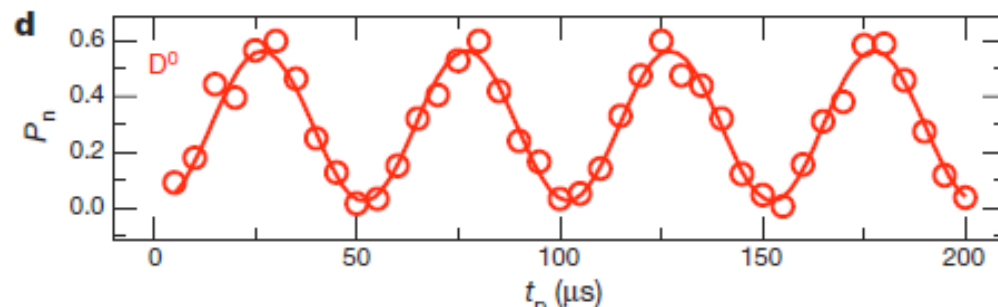
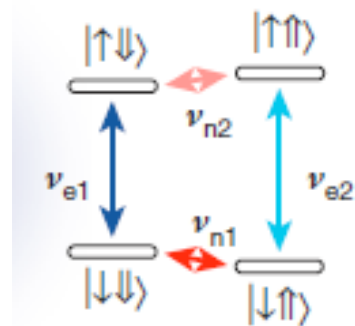
Problem: Existing theory consider bulk systems.
 → Need to include the effect of E-fields.

1998: Proposal



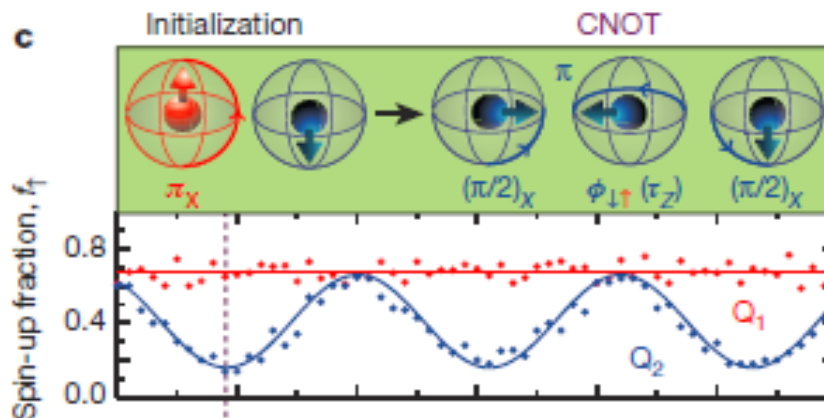
Kane, Nature 393, 133 (1998)

2013: Demonstration of a single qubit operation

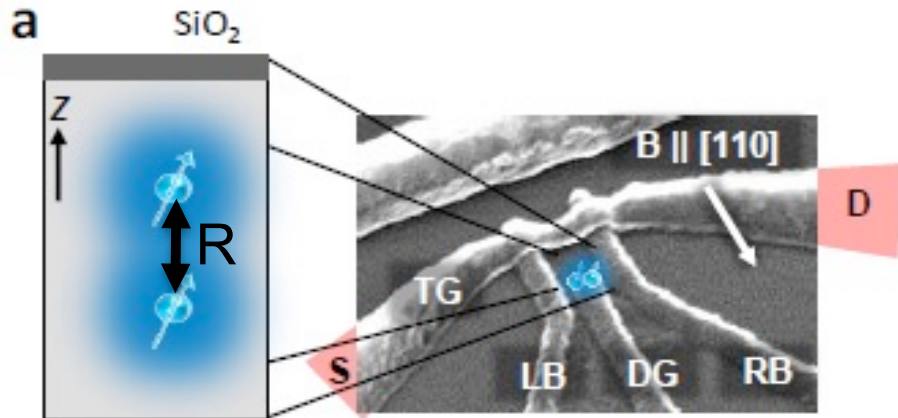


Pla, Nature 496, 334 (2013)

Next step: two-qubit logic gate



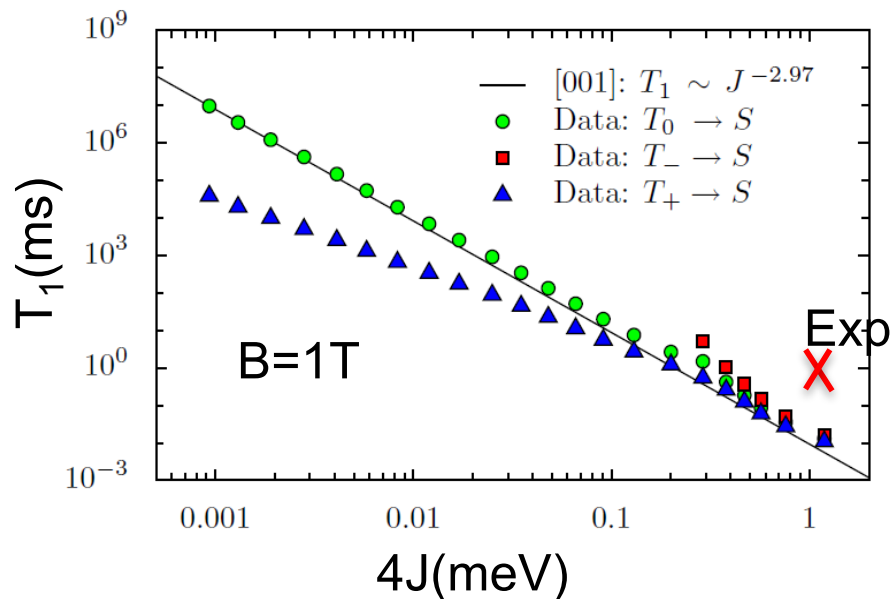
Veldhorst, Nature 526, 410 (2015)



Measurement:

→ $T_1 \sim 4\text{ms}$ at $B=0\text{T}$, $R \sim 6\text{nm}$.

→ Weak B dependence.



Existing work:

→ $T_1 \sim 0.01\text{ms}$ at $B=0\text{T}$, $R \sim 6\text{nm}$.

Problem: Existing work cannot explain measurements.

→ Need an accurate way to treat the two-electron T_1 problem.

J. P. Dehollain, et al., Phys. Rev. Lett. **112**, 236801 (2014).

M. Borhani and X. Hu, Phys. Rev. B **82**, 241302 (2010).

Introduction to quantum computing and T_1

The spin-relaxation mechanisms : Existing theories

Part I: The tight-binding T_1 method

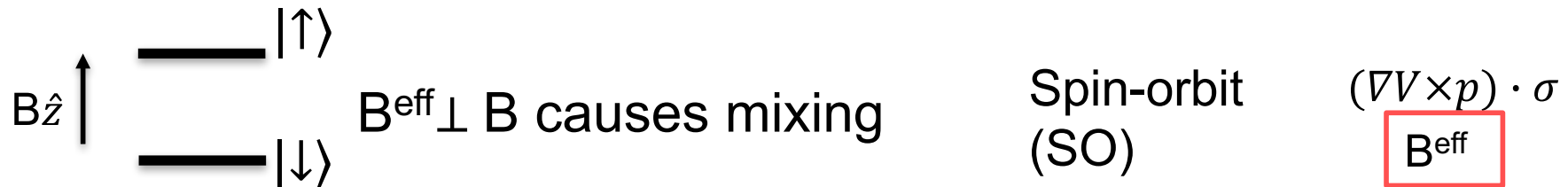
Part II: T_1 in device with electric fields

Part III: Two-electron T_1 problem

How does the electron relax to its lower energy state?

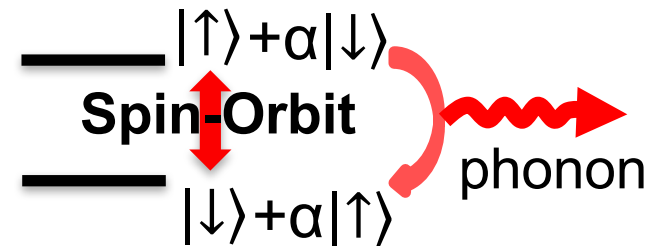
Transition between two energy states needs

1. a non-vanishing matrix element which connects them.

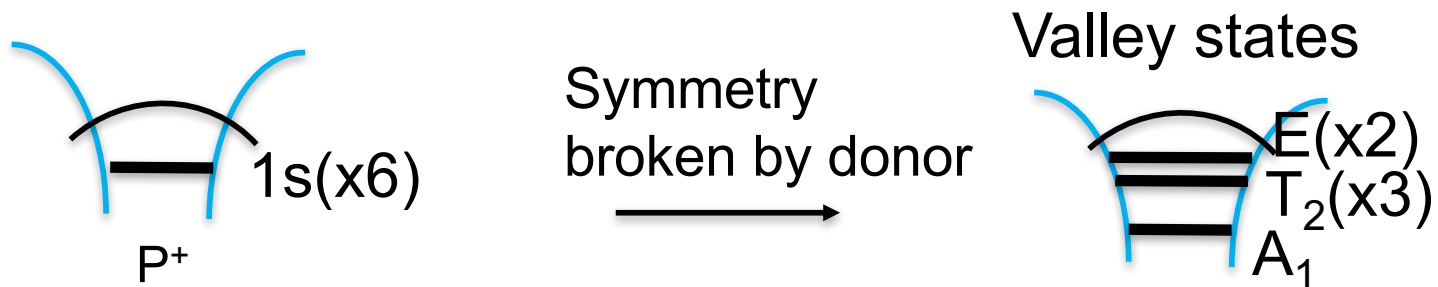


2. a time-dependent interaction.

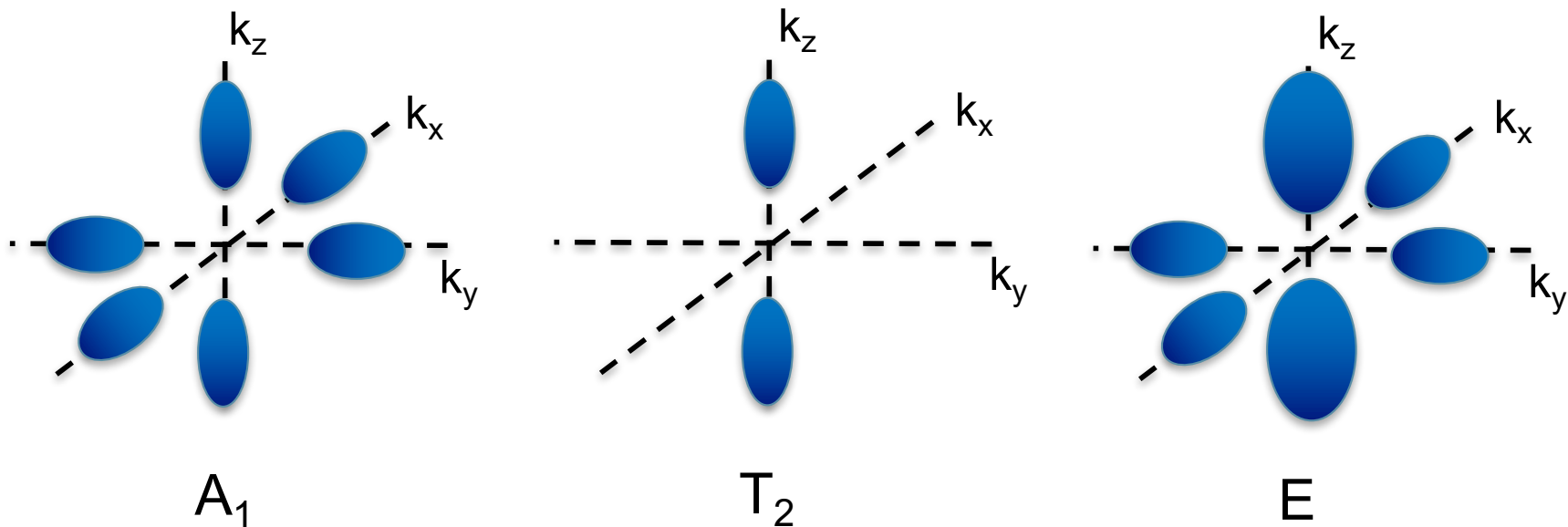
→ Electron-phonon interaction (H_{ep})



Si crystal provides spin-orbit and phonons which form a spin-relaxation channel



Example of valley compositions

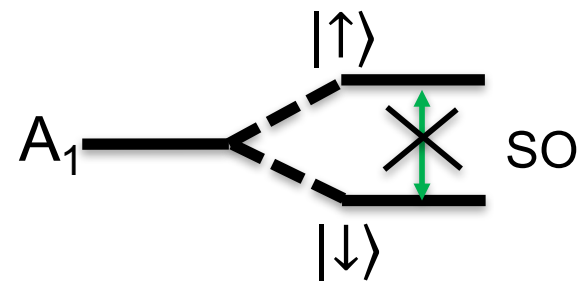
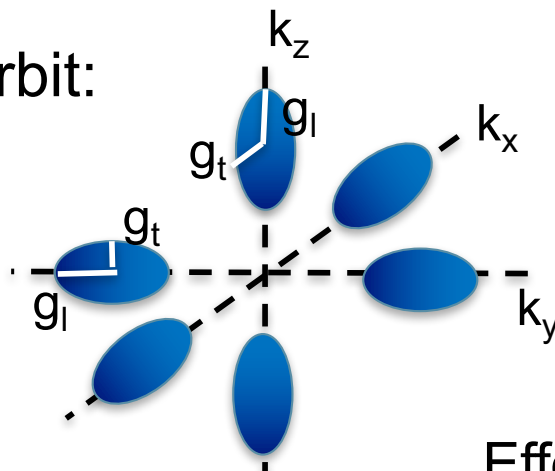


The donor states have different valley configurations.

The effect of spin-orbit:

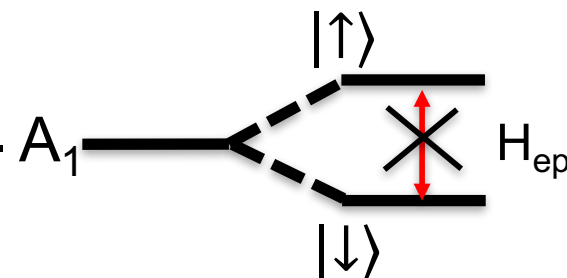
$$H_Z = g\mu_B B \cdot \sigma$$

g_l g_t



Effect of SO averaged out.

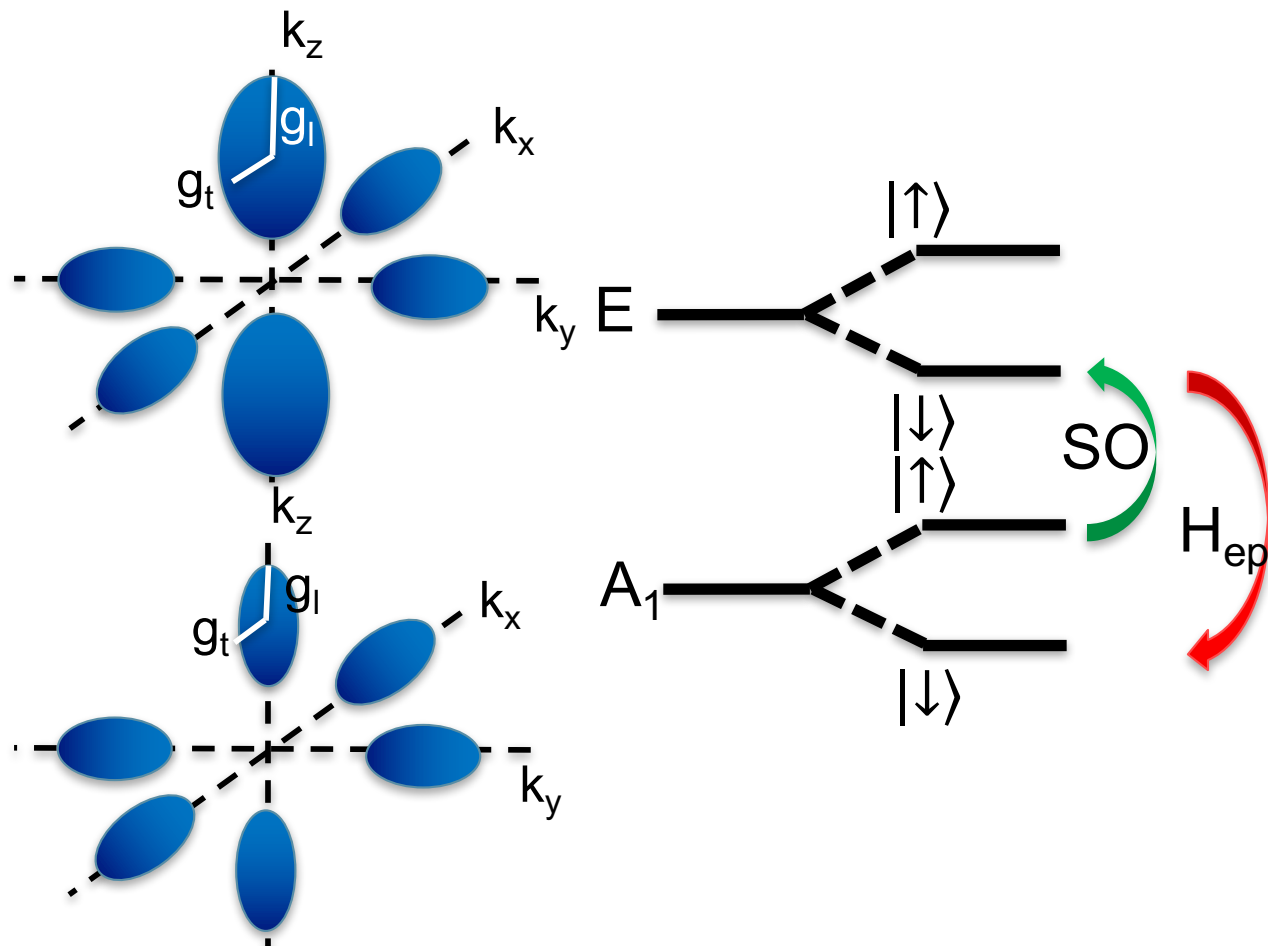
Phonon cannot change electron spins directly.



No direct way for the electron to relax.

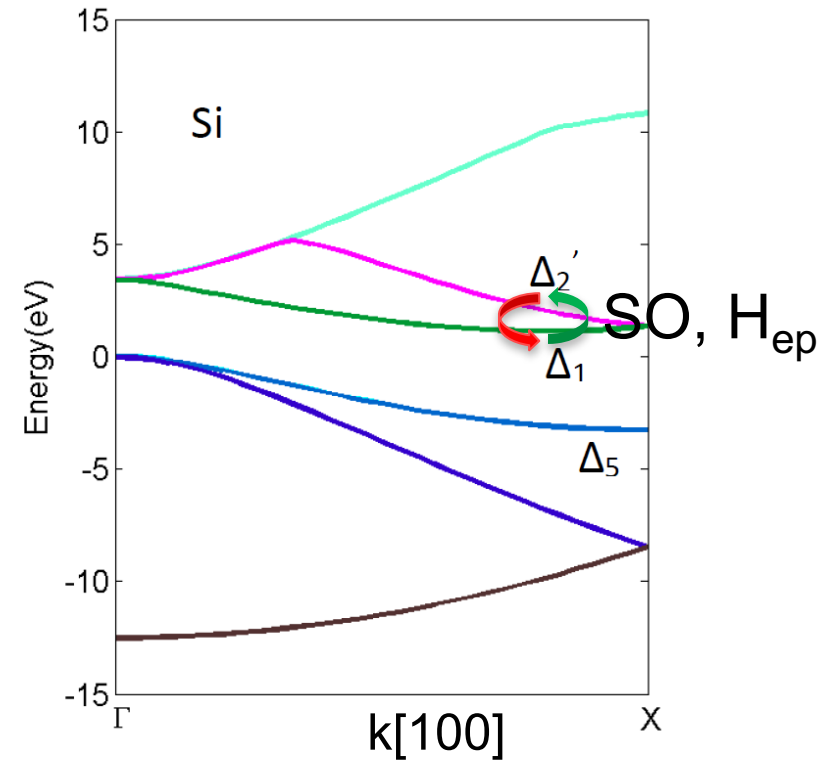
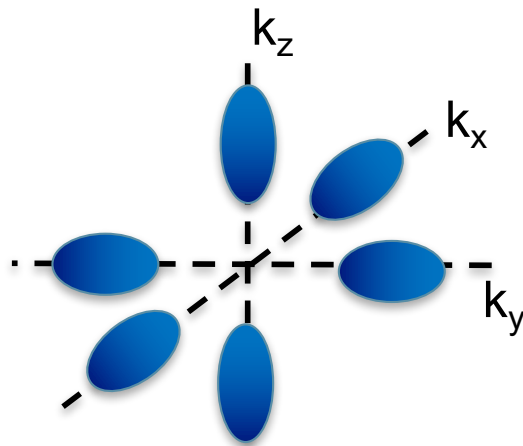
The effect of spin-orbit:

$$H_Z = g\mu_B B \cdot \sigma$$



Spin-orbit couples different valley states, a spin-relaxation channel is formed.

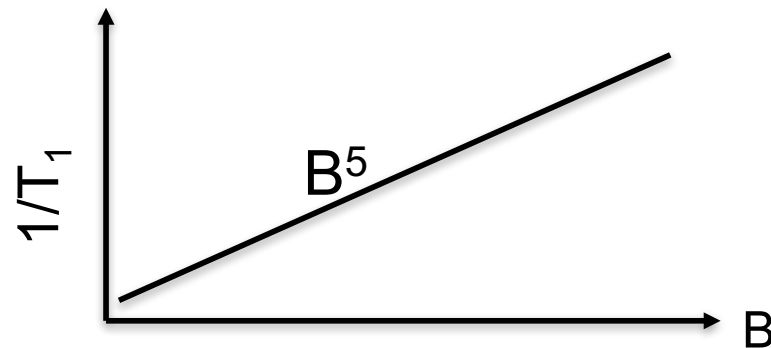
For a single valley...



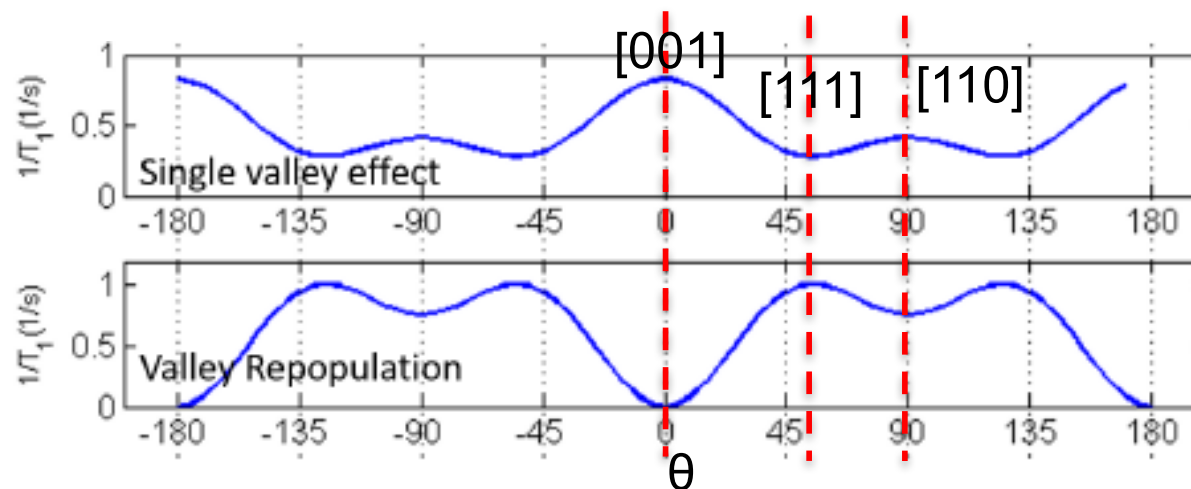
Electron relaxes through mixing with higher-lying conduction bands around each valley.

- Magnitude
 $1/T_1 \sim 1\text{s}$ for $B=3.5\text{T}$, $T=100\text{mK}$,

- B dependence



- Anisotropy



Existing theories consider T_1 of single donors in bulk Si, have $1/T_1 \sim B^5$ and peaks at $B//[111]$.

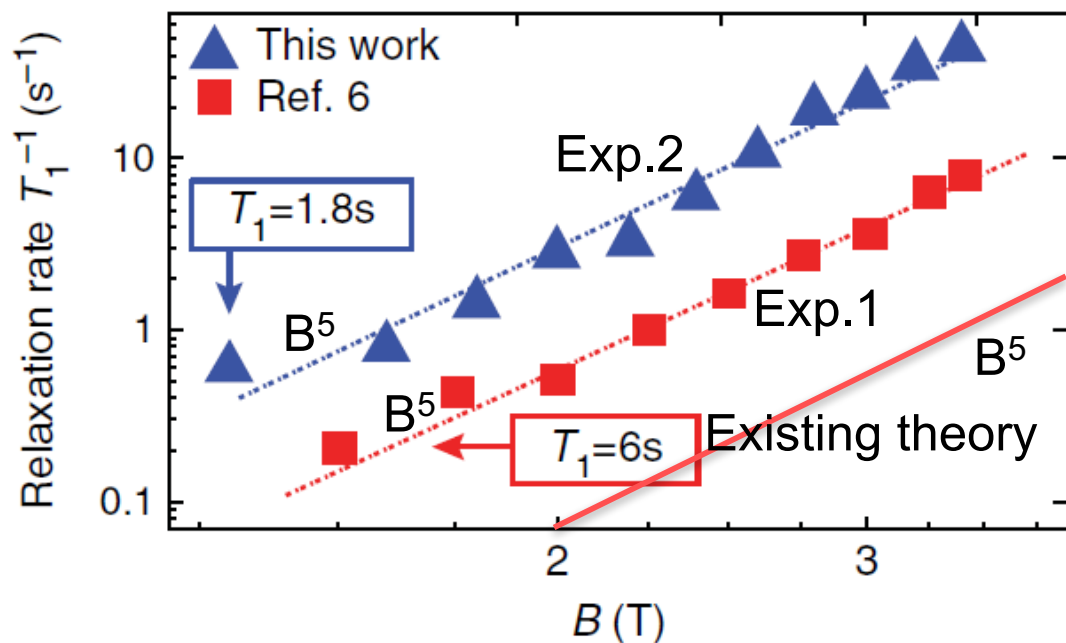
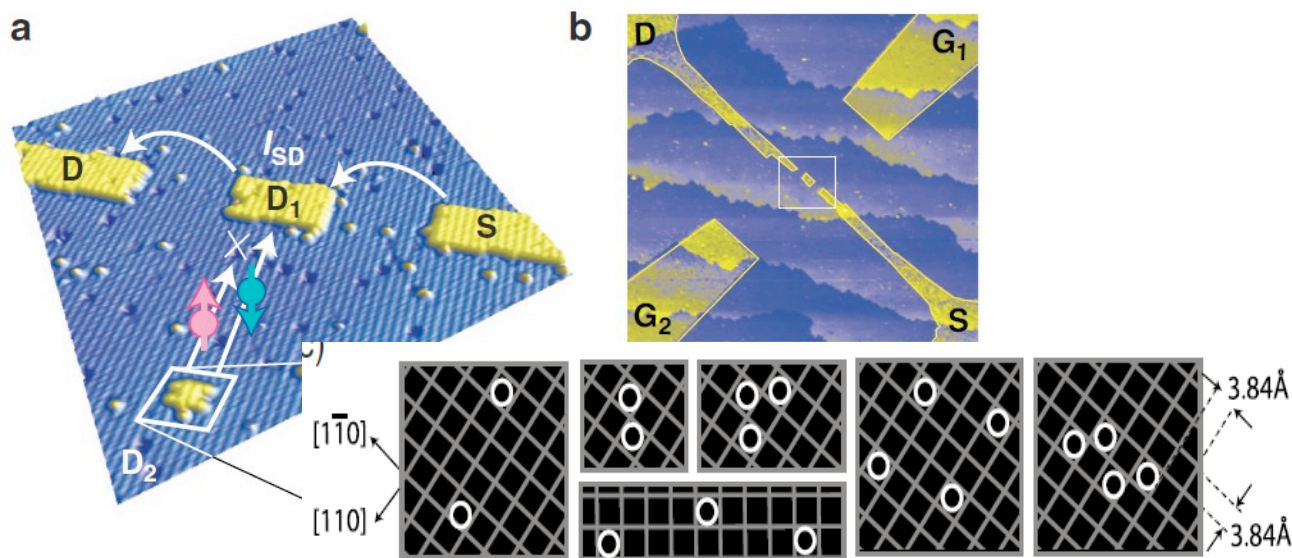
Introduction to quantum computing and T_1

The spin-relaxation mechanisms : Existing theories

Part I: The tight-binding T_1 method

Part II: T_1 in device with electric fields

Part III: Two-electron T_1 problem



Problem: Existing theories only consider single donors.
 → Need a comprehensive approach to calculate T_1 in donors and donor clusters.

The phonon modes involved

Acoustic phonon → deformation potential theory

Existing theories:

Valley repopulation:

- effective mass wf. with valleys
- H_{ep} :
diagonal strain (u_{xx}, u_{yy}, u_{zz})
exp. input: deformation potential constants

Single valley:

- H_{ep} :
off-diagonal strain (u_{xy}, u_{xz}, u_{yz})
exp. input: matrix element

A comprehensive approach for T_1

- TB wf.
- H_{ep} :
strained TB Hamiltonian

$$\hat{H}_{ep} = \sum_{i,j=x,y,z} \hat{\Xi}_{ij} u_{ij},$$

$$\hat{\Xi}_{ij} = \frac{\partial \hat{H}_e}{\partial u_{ij}} = \frac{\hat{H}_e(u_{ij}) - \hat{H}_e(0)}{u_{ij}}$$

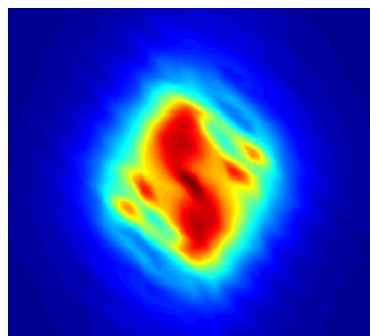
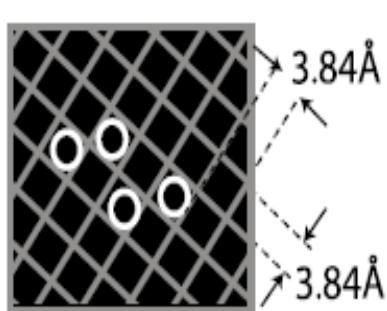
→ captures both valley repopulation and single valley effects.

→ valley information not needed

→ no exp. input

The atomistic TB Hamiltonian

- spin-orbit interaction
- magnetic field
- self consistent TB



Computed outermost
electron wf. of 4P5e

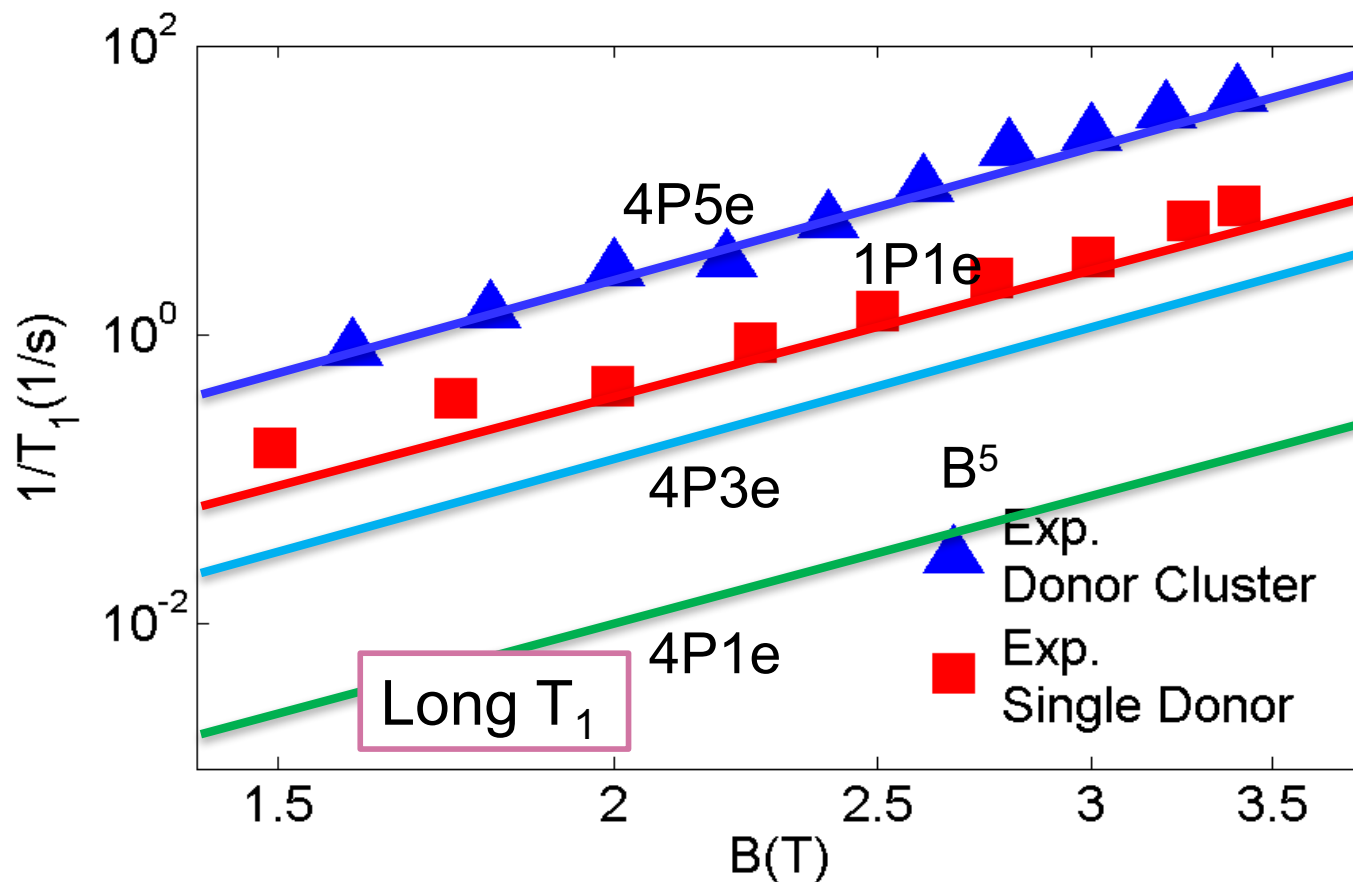
The T_1 time

- Deformation potentials for all strain components from strain-dependent TB Hamiltonian
- Strain: bond distortion

A diagram illustrating bond distortion. On the left, three spheres are connected in a straight line. On the right, the same three spheres are shown with the central one displaced, forming an angle θ between the bonds.
- Fermi's Golden rule for $1/T_1$

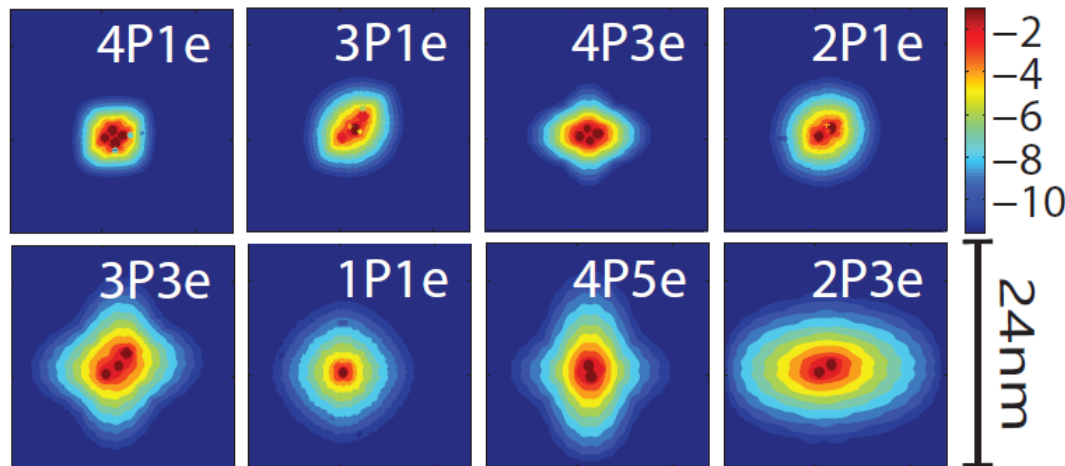
Atomic basis captures critical physics of
spin-orbit interactions and bond distortions.

4P5e: Donor cluster with 4 donors 5 electrons.



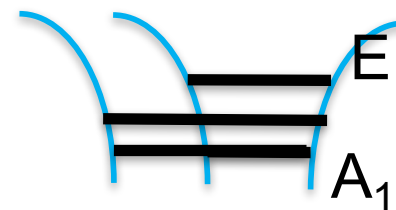
Electron number variation results in orders of magnitude change in T₁

H. Büch et al. Nature Communications 4, 2017 (2013)
Y. L. Hsueh et al., Phys. Rev. Lett. 113, 246406 (2014)

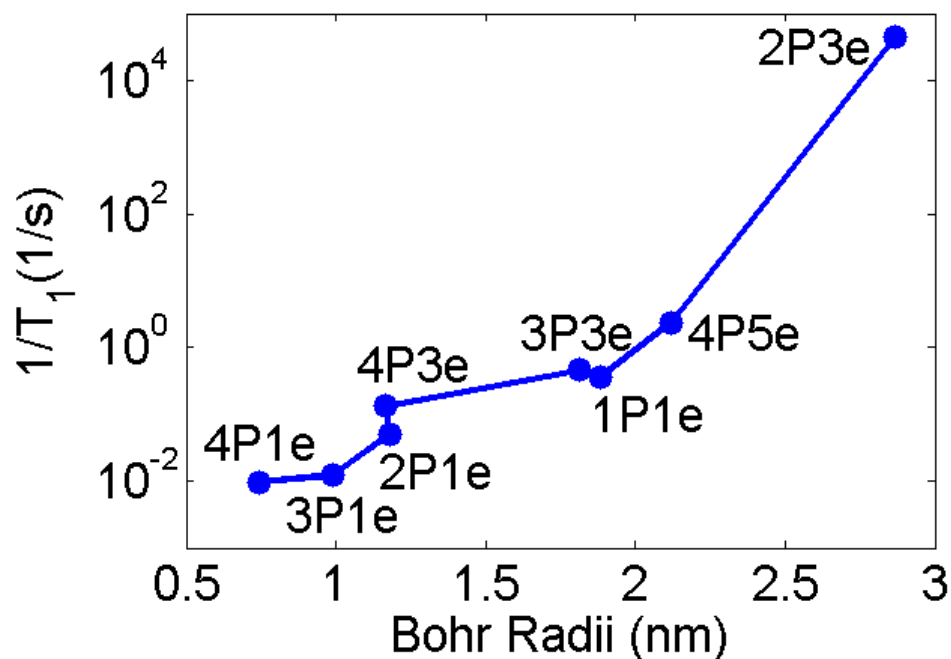


The computed wf (in log scale).

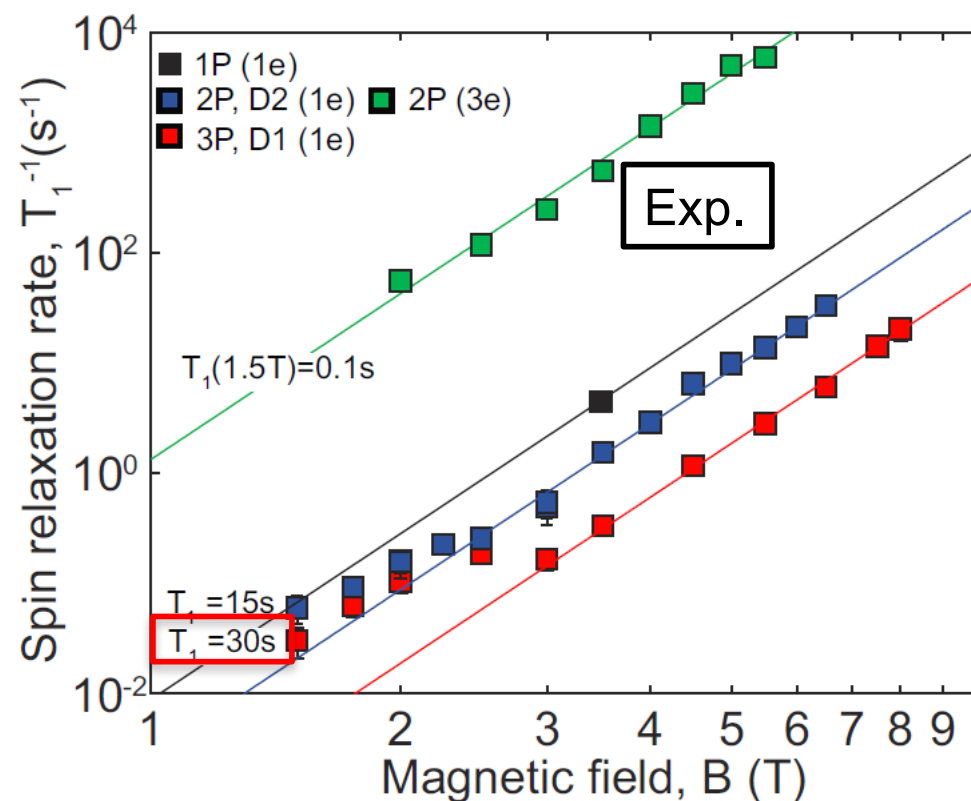
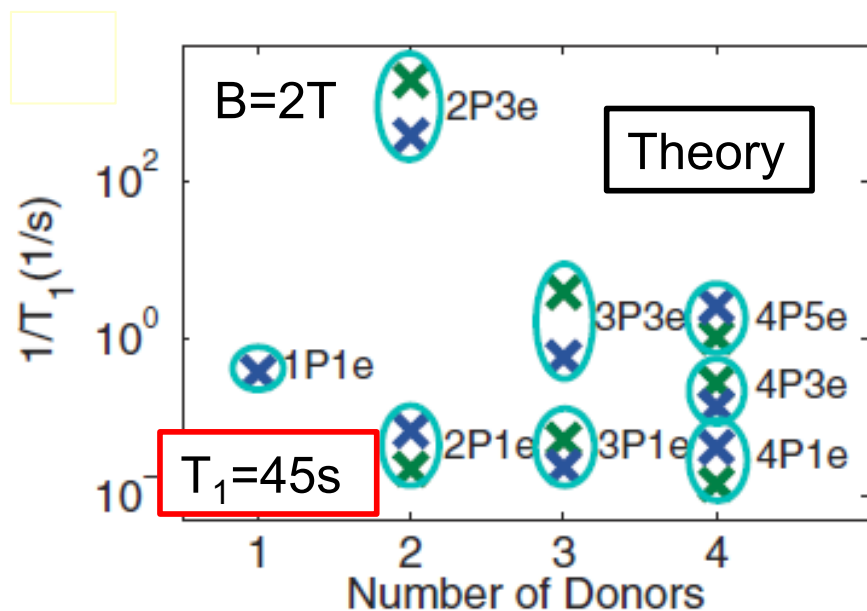
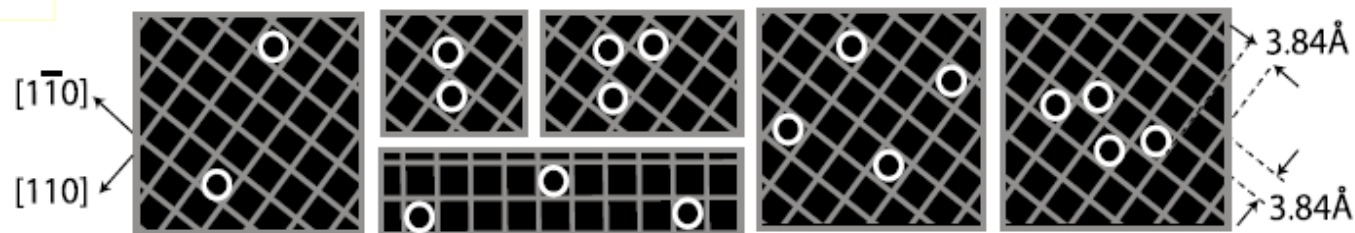
Valley states



Large electron wf
 \rightarrow valley states are closer
 \rightarrow large $1/T_1$

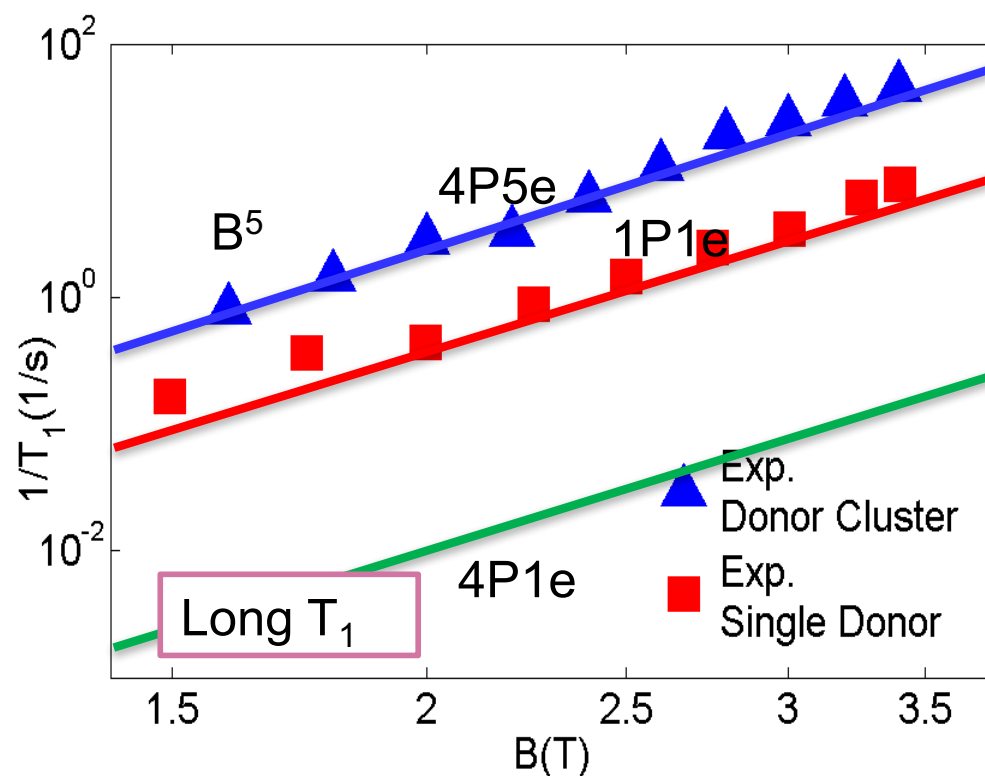


Small electron Bohr radius
 results in long T_1 time.



Experimental results confirmed our theoretical prediction.

- A TB method is benchmarked with recent exp. observation.
- Long T_1 times in donor clusters are predicted and confirmed.



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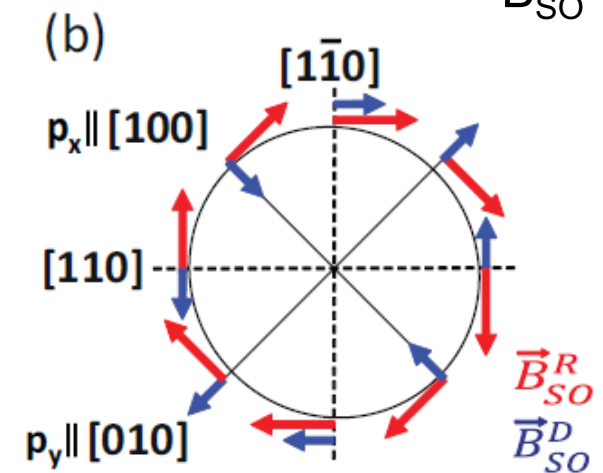
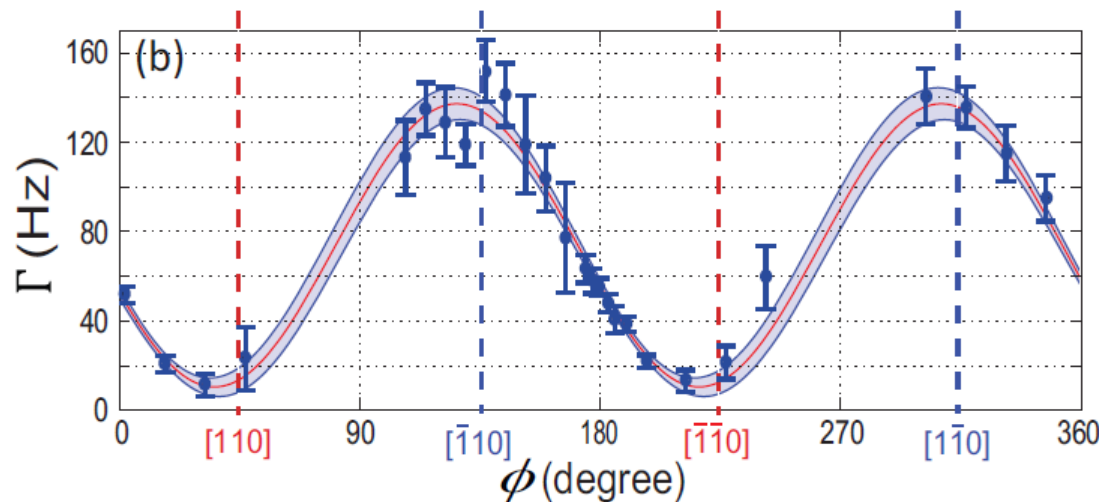
Part III: Two-electron T_1 problem

GaAs \rightarrow bulk inversion asymmetry \rightarrow **Dresselhaus SO**

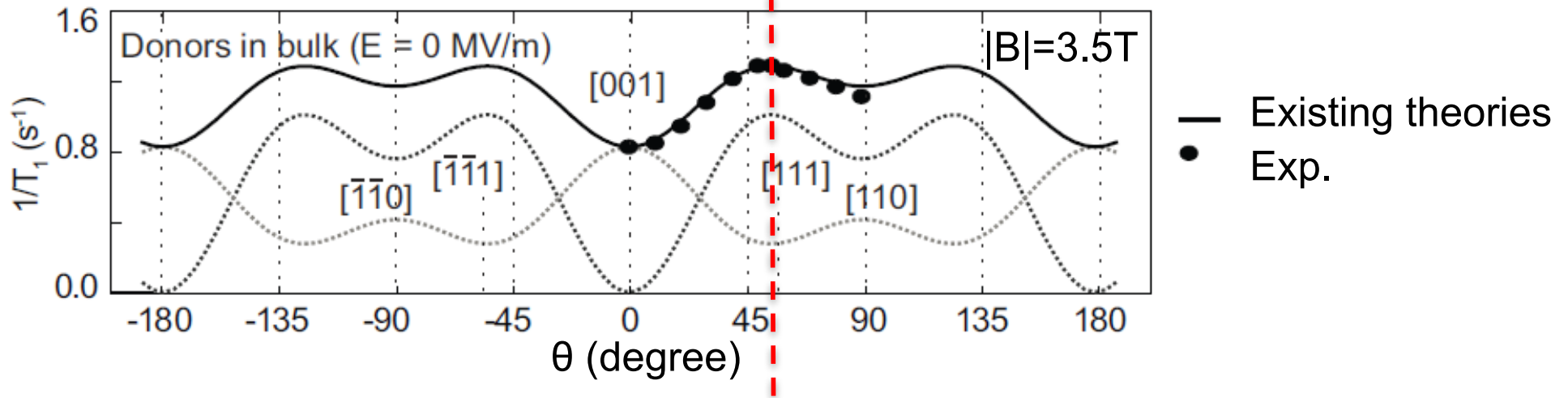
QDs \rightarrow structural inversion asymmetry (E field) \rightarrow **Rashba SO**

Question: the sign of Rashba and Dresselhaus?
 \rightarrow Extract from T_1 anisotropy

$$H_{so} = \sigma \cdot \underbrace{\beta(k \times \hat{E})}_{B_{SO}}$$



We can extract information about the spin-orbit interaction from measuring T_1 anisotropy.

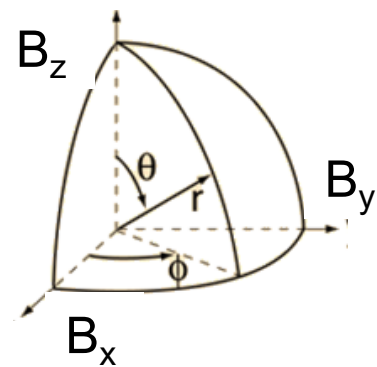


Bulk Si \rightarrow no Dresselhaus SO

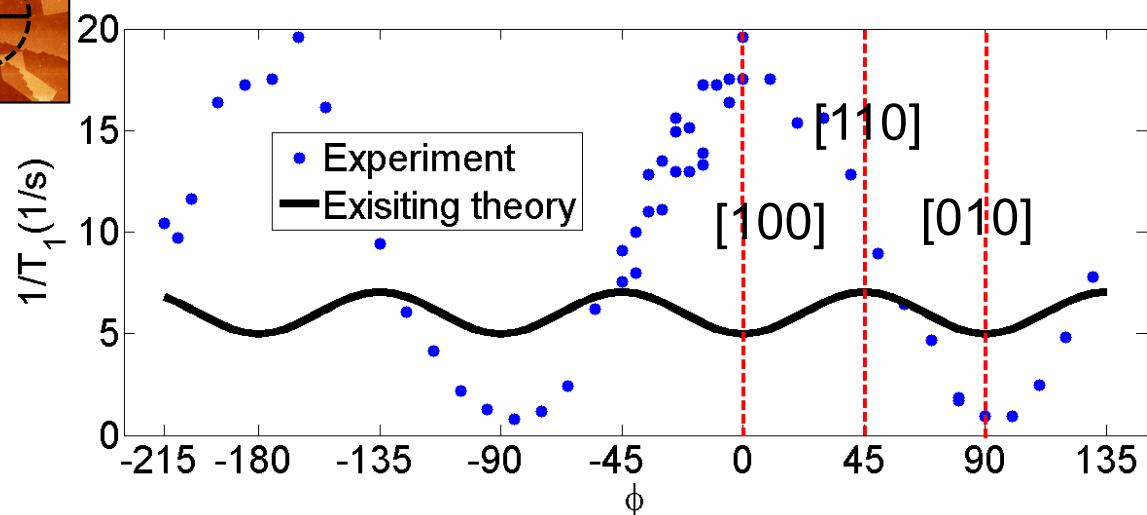
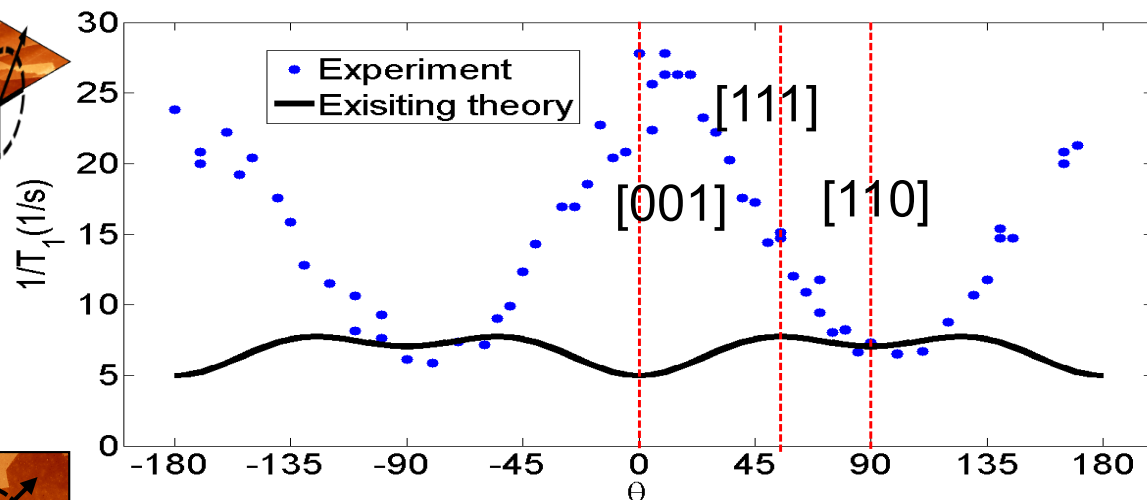
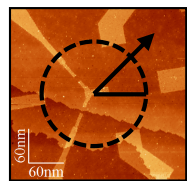
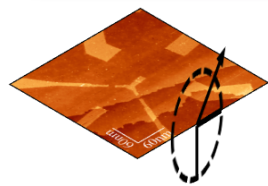
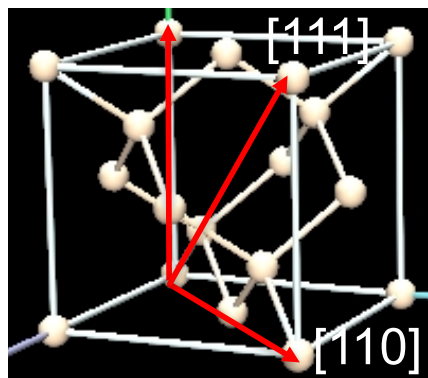
No E field \rightarrow no Rashba SO

Only spin-orbit from the crystal $H_{so} = \sigma \cdot (\nabla V \times p)$

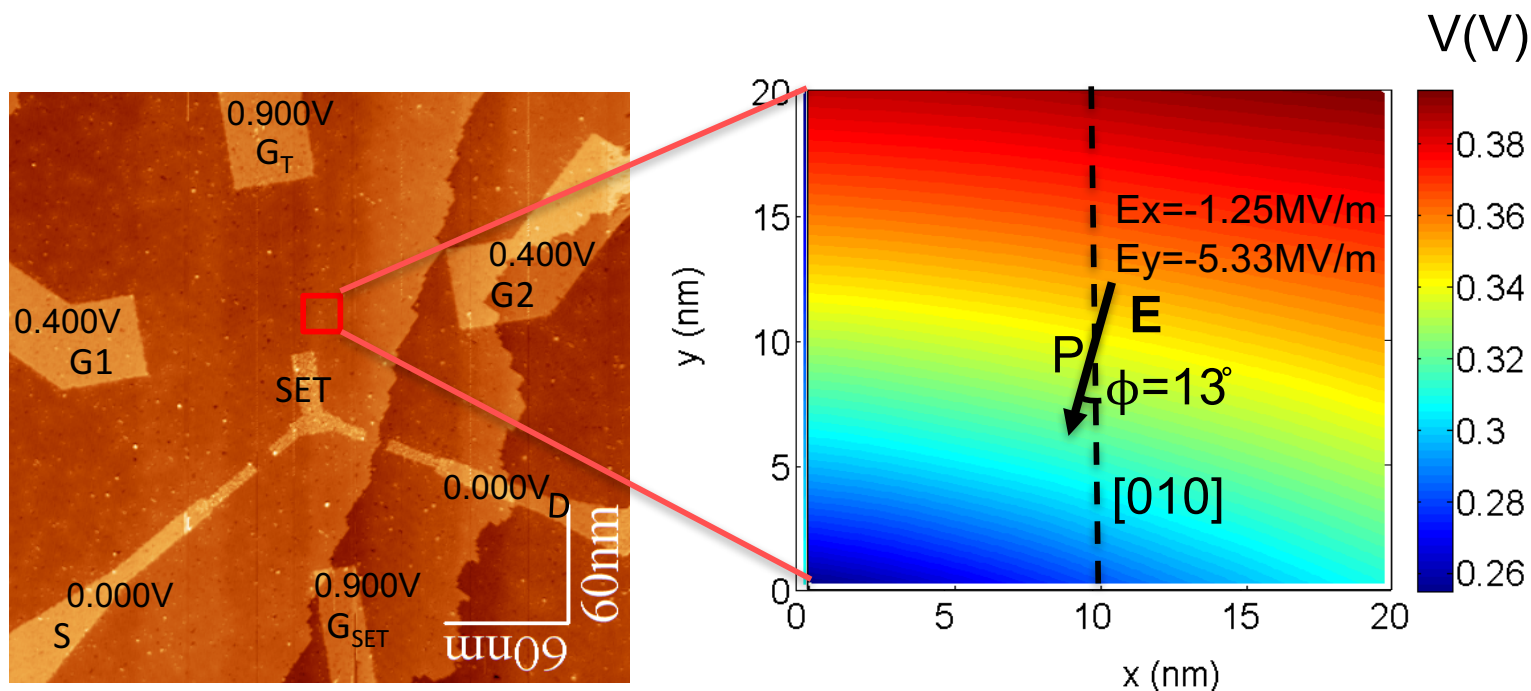
Bulk P in Si: T_1 anisotropy follows crystal symmetry, and is explained by existing theories.



[001]



Problem: Existing theory considers bulk systems.
 → Need to include the effect of E-fields.



Electrostatics solved from COMSOL

Electric field ($E_y \sim 5 MV/m$) at the donor site.

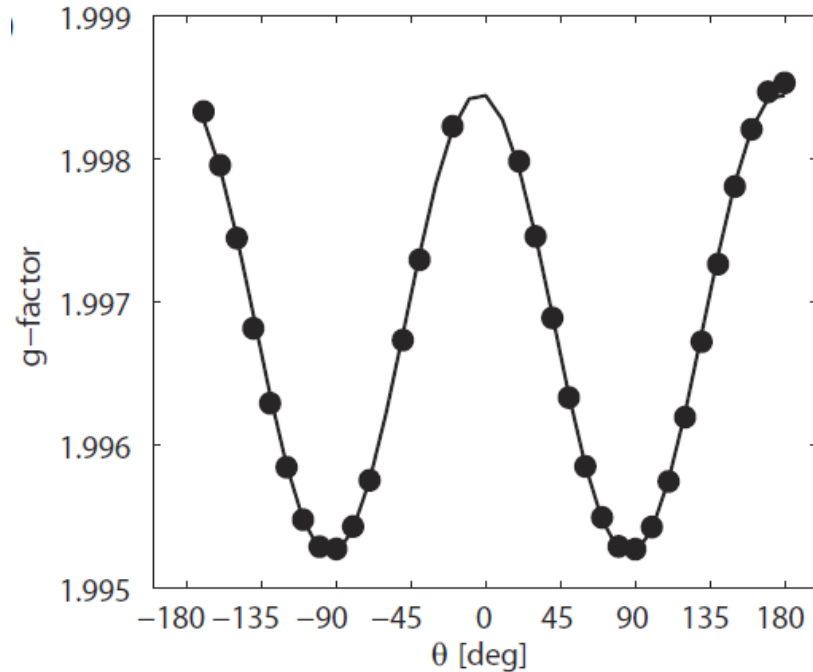
Rashba spin-orbit

$$H_{SO} = R(\mathbf{k} \times \mathbf{E}) \cdot \boldsymbol{\sigma}$$

$$H_Z = \underbrace{g_l}_{\text{Bulk SO}} \mu_B B \cdot \boldsymbol{\sigma} + \underbrace{R(\mathbf{k} \times \mathbf{E}) \cdot \boldsymbol{\sigma}}_{\text{Rashba SO}}$$

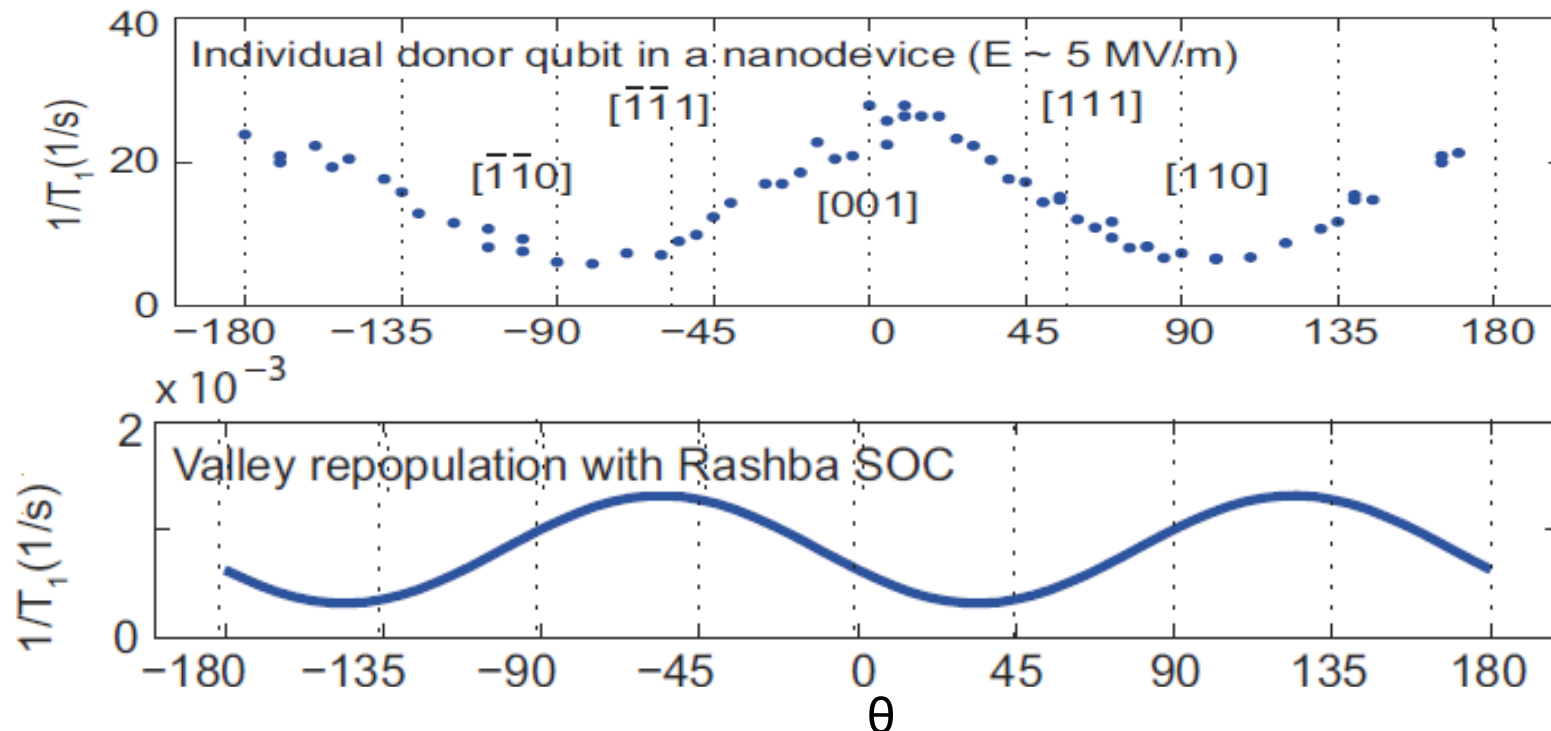
$$\equiv g \mu_B B$$

- Analytic expression
- Tight-binding calculations



Fit to TB g factor → Rashba $B_{\text{eff}} \sim 0.1 \text{ mT}$ Electron g-factor of donor in Si

From spin-splitting → extract the magnitude of Rashba SO in donors.



Under E field along y,
 $B^{\text{eff}} // [101] \rightarrow$ maximum mixing at $B \perp [101]$

Valley repopulation with Rashba SO cannot explain the observed anisotropy.

Beyond the usual spin-orbit, we consider the next higher-order term in $k \cdot p$ theory

$$H_{so} = C(\mathbf{E} \times \mathbf{B})^+ \cdot \boldsymbol{\sigma}$$

- Couples the external electric and magnetic field.
- No orbital dependence.
- \mathbf{E} along $[010]$, $\mathbf{B} // \mathbf{E} \rightarrow H_{so} = 0$, $\mathbf{B} \perp \mathbf{E} \rightarrow H_{so}$ largest

A new SO coupling having $(\mathbf{E} \times \mathbf{B})^+$ form might be present.

Note: $(\mathbf{E} \times \mathbf{B})^+ = (E_y B_z + E_z B_y, E_x B_z + E_z B_x, E_x B_y + E_y B_x)$

R. Winkler et al., Spin-Orbit Coupling in Two-Dimensional Electron and Hole Systems.

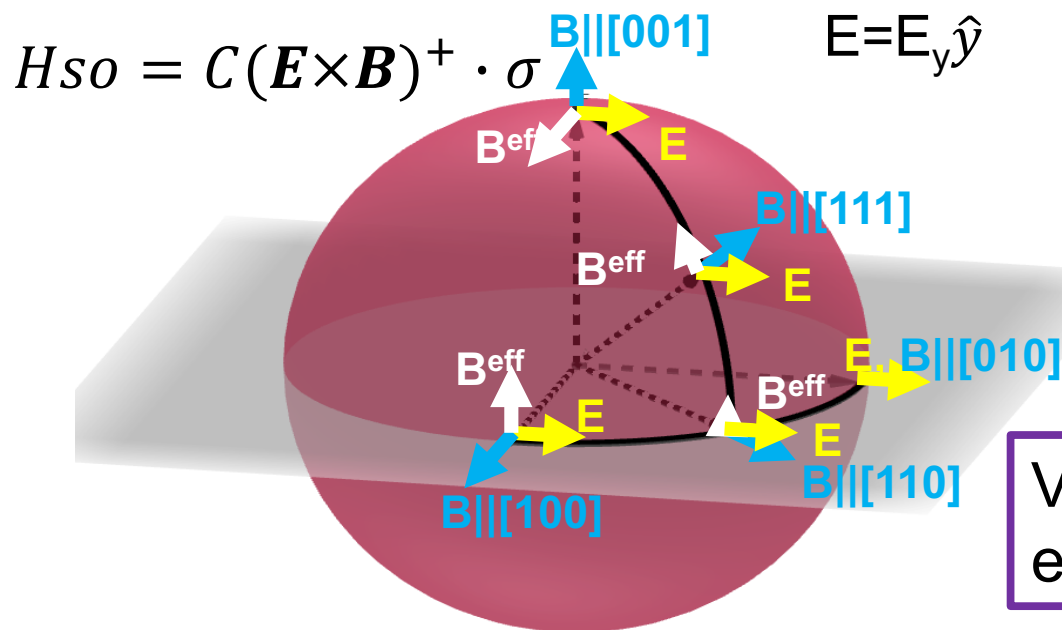
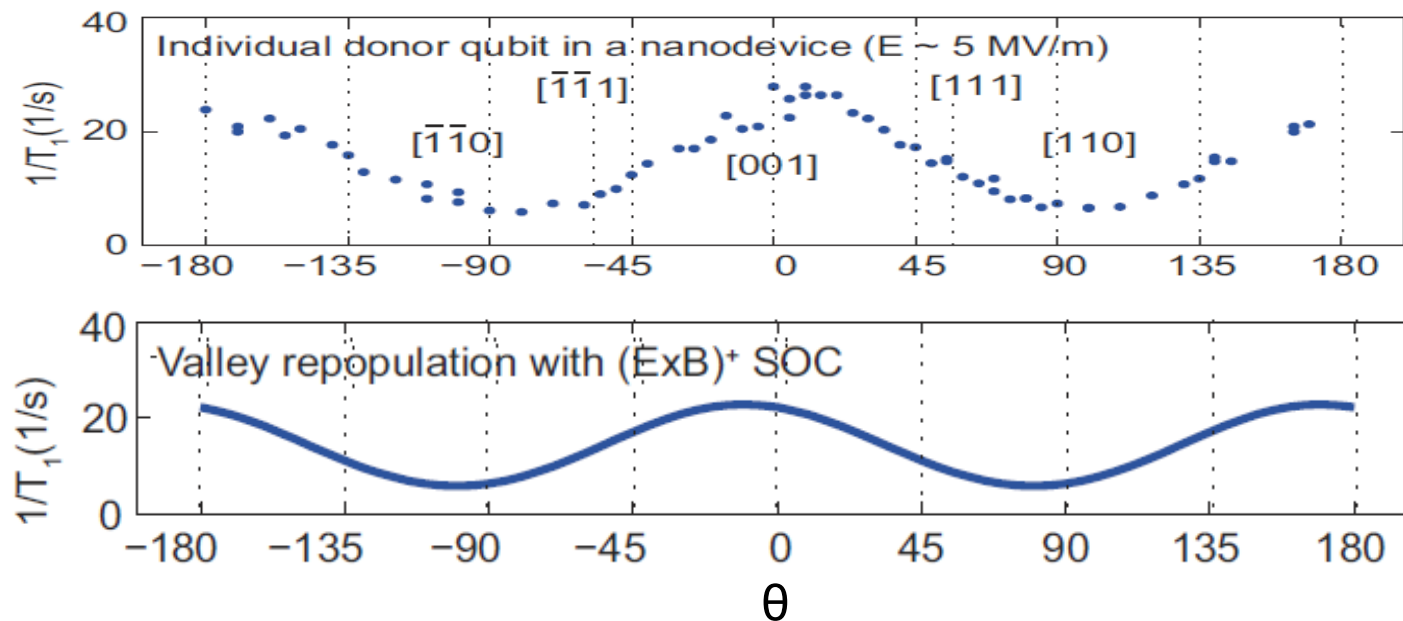
$$\frac{C}{R} = \frac{e}{m_0} \frac{p_{\mu\nu}}{E_{\alpha\mu}}$$

Rashba spin-orbit $H_{SO} = R(\mathbf{k} \times \mathbf{E}) \cdot \boldsymbol{\sigma}$ \rightarrow Rashba $B_{\text{eff}} = 0.1 \text{ mT}$

H_{ExB} spin-orbit $H_{SO} = C(\mathbf{E} \times \mathbf{B})^+ \cdot \boldsymbol{\sigma}$ \rightarrow H_{ExB} $B_{\text{eff}} = 18.9 \text{ mT}$

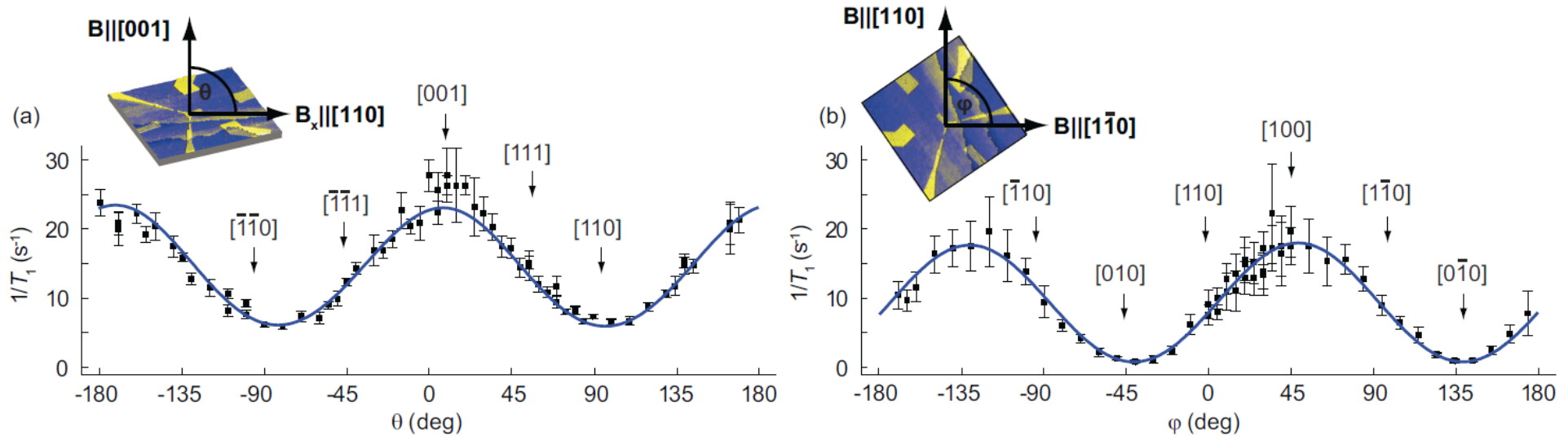
Why Rashba smaller? $R > C$, but k very small in donors.

From comparing to Rashba SO
 \rightarrow extract the magnitude of H_{ExB} SO in donors.



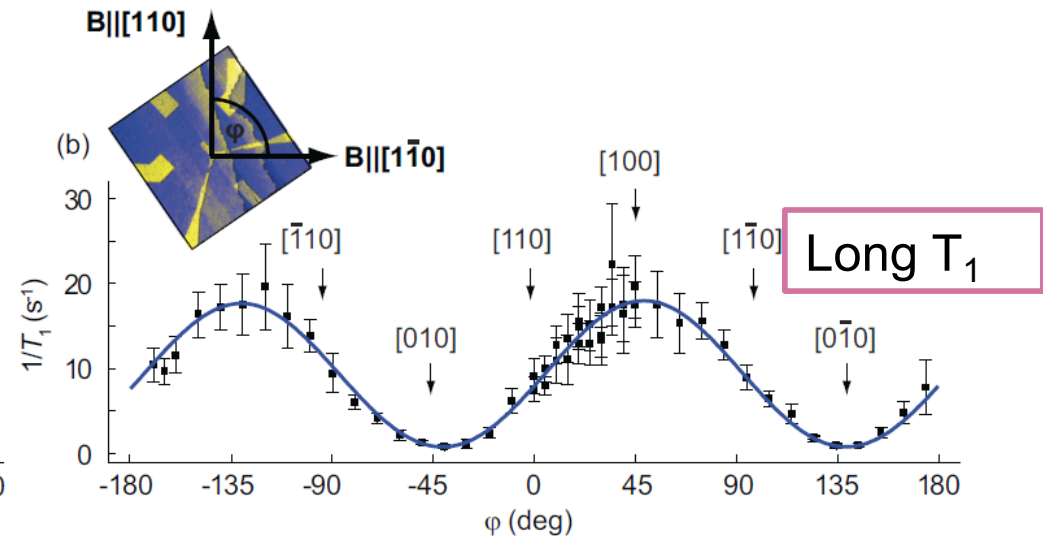
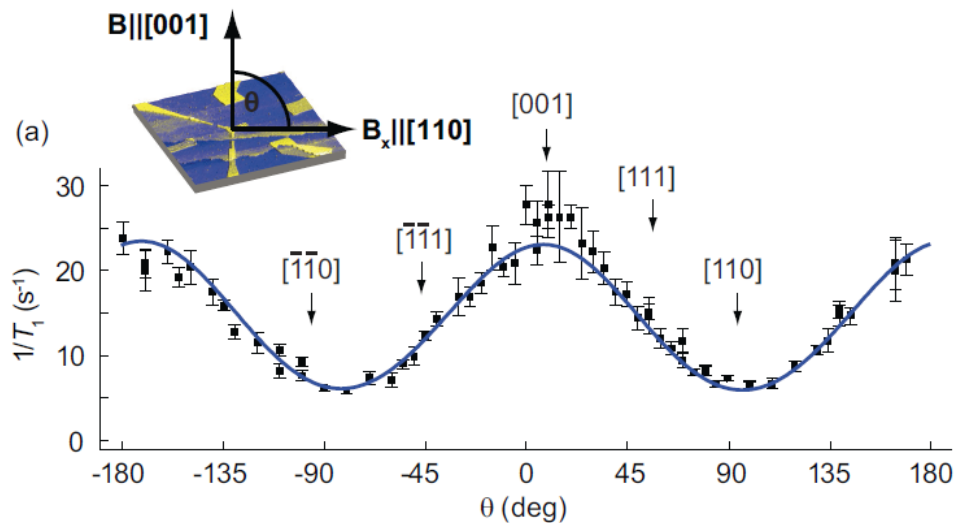
Under E field along y ,
 B^{eff} is largest along $[001]$.

Valley repopulation with $(E \times B)^+ \text{ SO}$
explains the observed anisotropy.



The T_1 anisotropy in a nano device is explained by electric field modified valley repopulation + single valley effect.

- A new electric field induced SO: H_{ExB} is found.
- The observed anisotropy is explained by the electric field-modified spin-relaxation mechanisms.



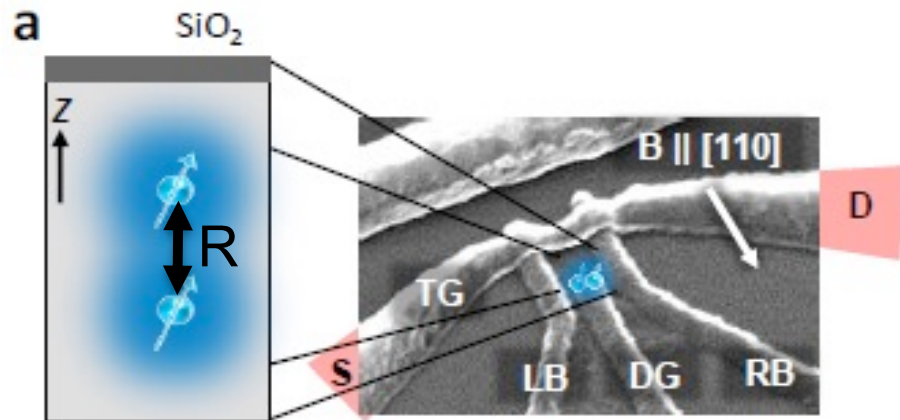
Introduction to quantum computing and T_1

The spin-relaxation mechanisms : Existing theories

Part I: The tight-binding T_1 method

Part II: T_1 in device with electric fields

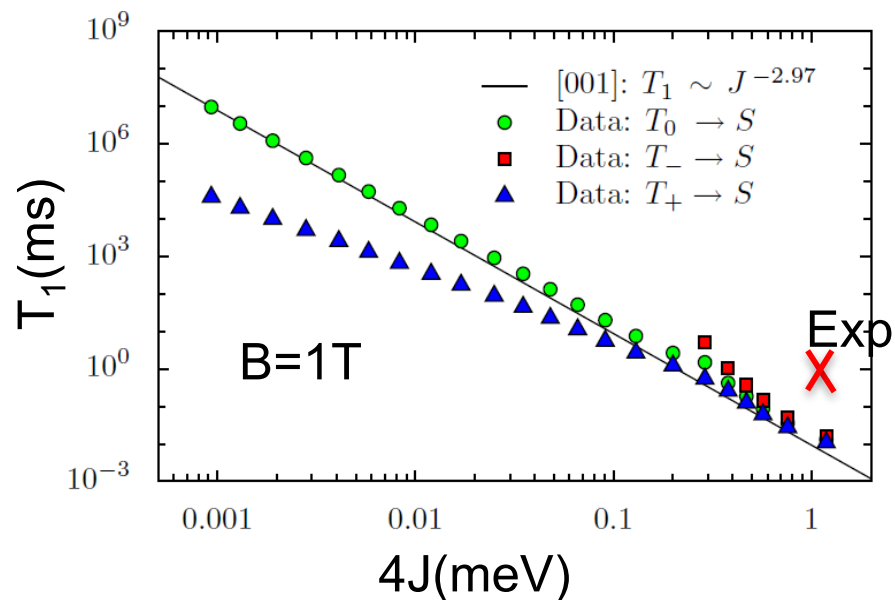
Part III: Two-electron T_1 problem



Measurement:

→ $T_1 \sim 4\text{ms}$ at $B=0\text{T}$, $R \sim 6\text{nm}$.

→ Weak B dependence.



Existing work:

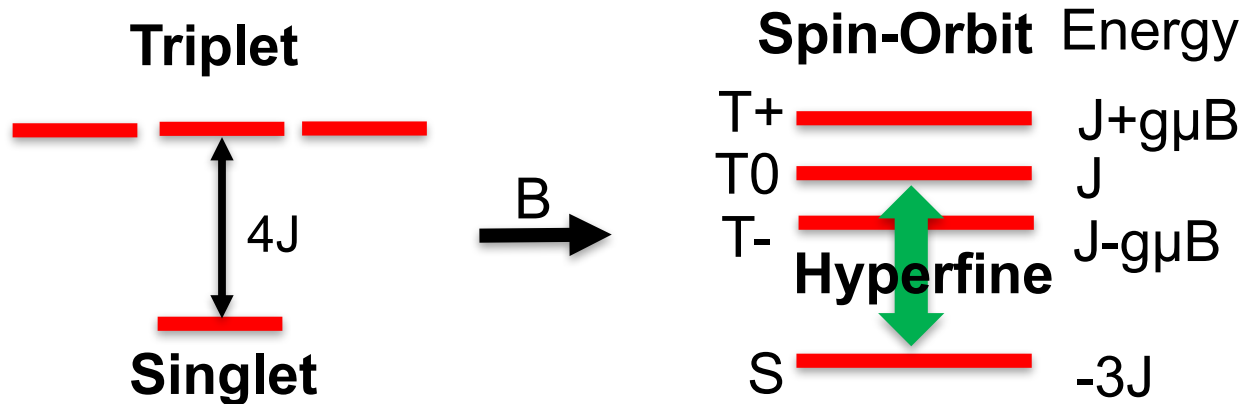
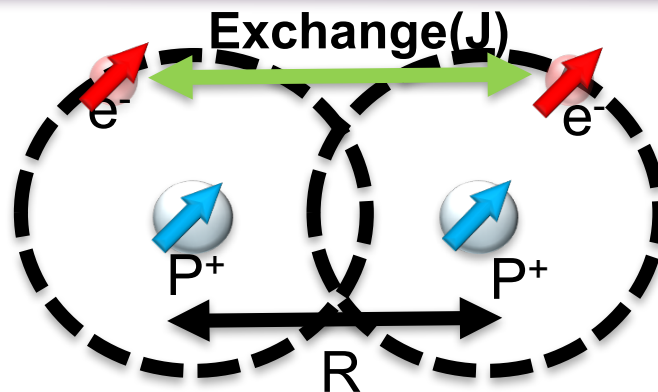
→ $T_1 \sim 0.01\text{ms}$ at $B=0\text{T}$, $R \sim 6\text{nm}$.

Problem: Existing work cannot explain measurements.

→ Need an accurate way to treat the two-electron T_1 problem.

J. P. Dehollain, et al., Phys. Rev. Lett. **112**, 236801 (2014).

M. Borhani and X. Hu, Phys. Rev. B **82**, 241302 (2010).



Goal

1. Calculate triplet to singlet T_1 due to SO and hyperfine mixing.
2. T_1 dependencies on J .

Fermi's Golden rule
$$\frac{1}{T_1} = \frac{2\pi}{\hbar} |\langle f | \hat{H}_{ep} | i \rangle|^2 \delta(E_i - E_f - \hbar\omega_q)$$

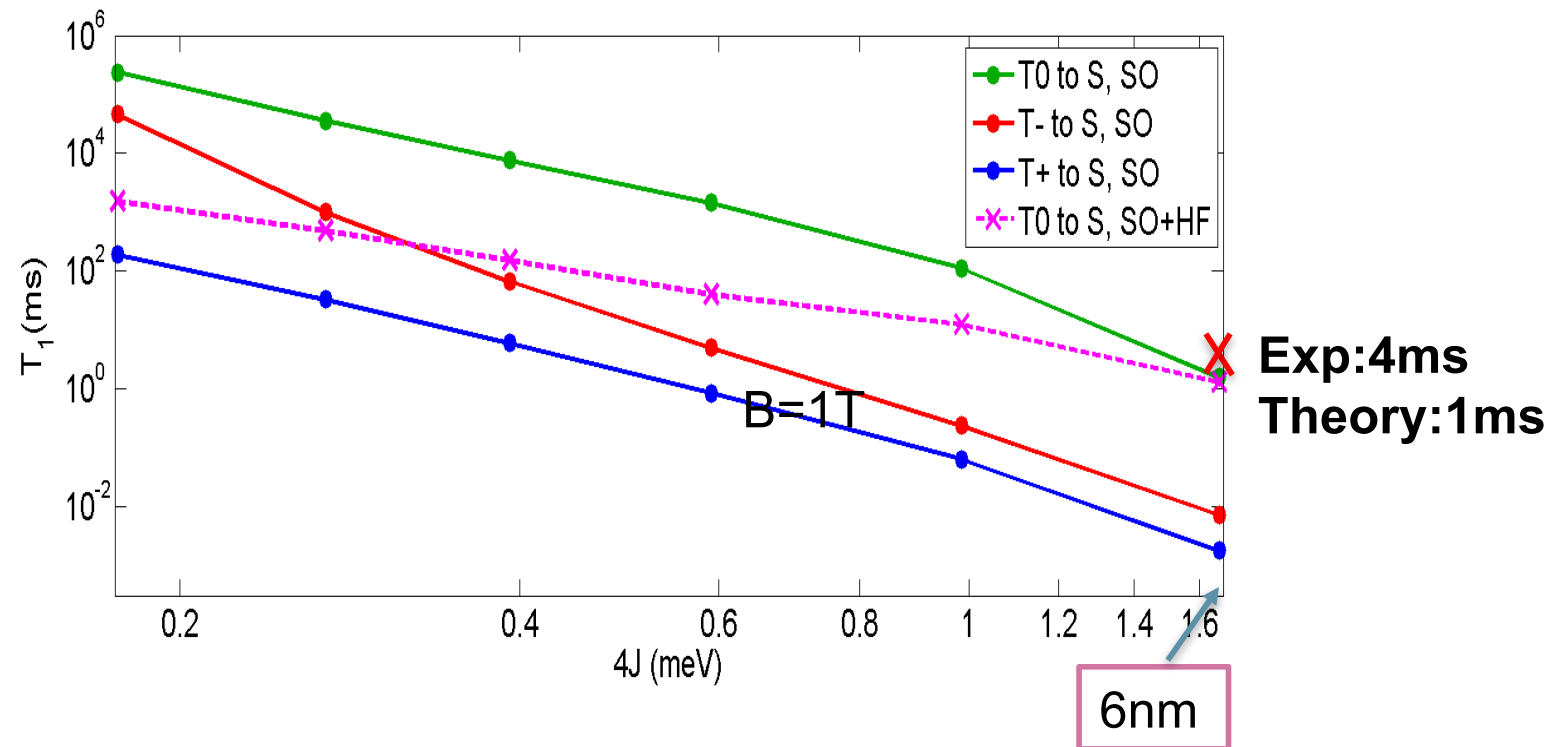
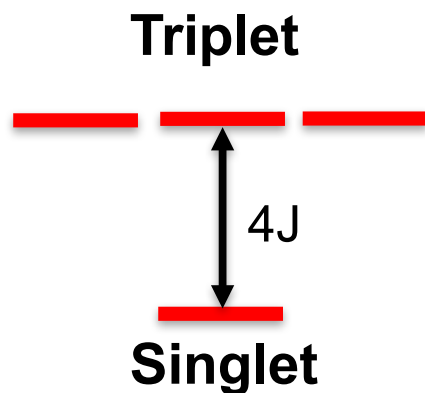
Existing work:

- $|i\rangle, |f\rangle$:
effective mass wf. with Heitler-London approximation.
- Hep:
deformation potential constants.
- Hyperfine mixing.

An accurate method:

- $|i\rangle, |f\rangle$:
Full-configuration interaction with slater determinants from one-electron TB wf.
- Hep:
strained TB Hamiltonian.
- Spin-orbit + hyperfine mixing.

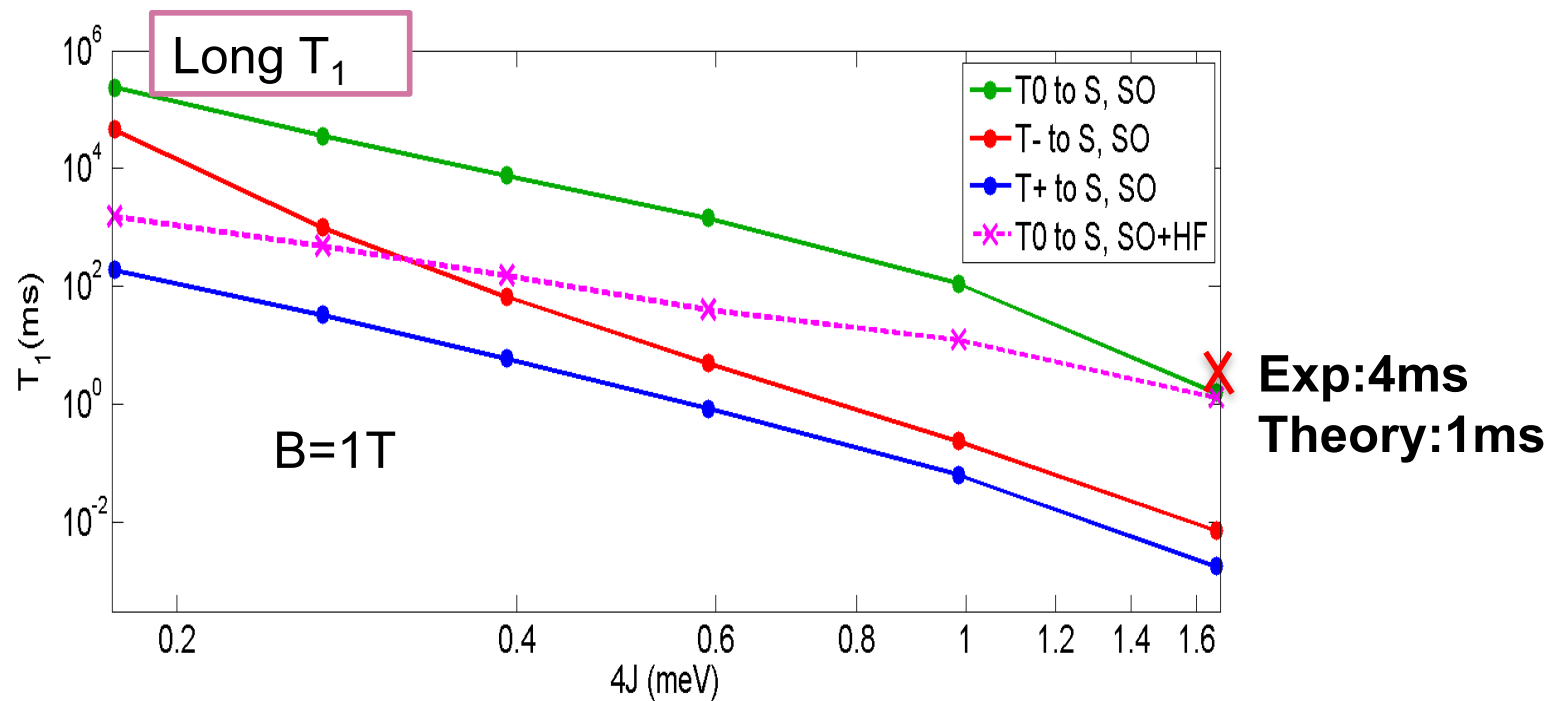
FCI + tight-binding to calculate 2e T₁.



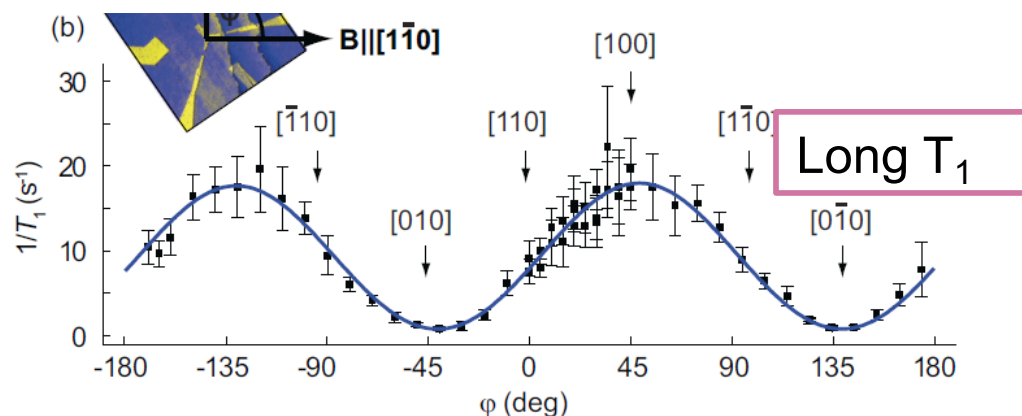
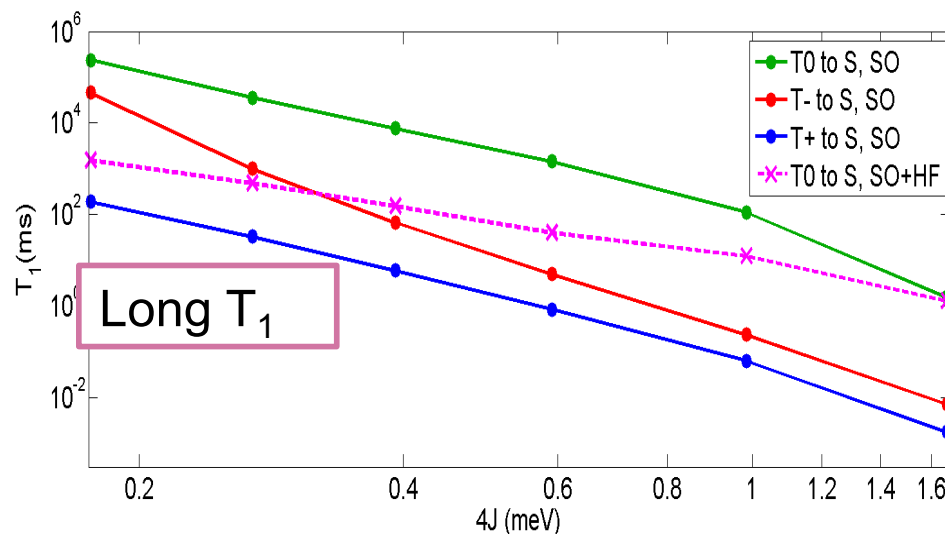
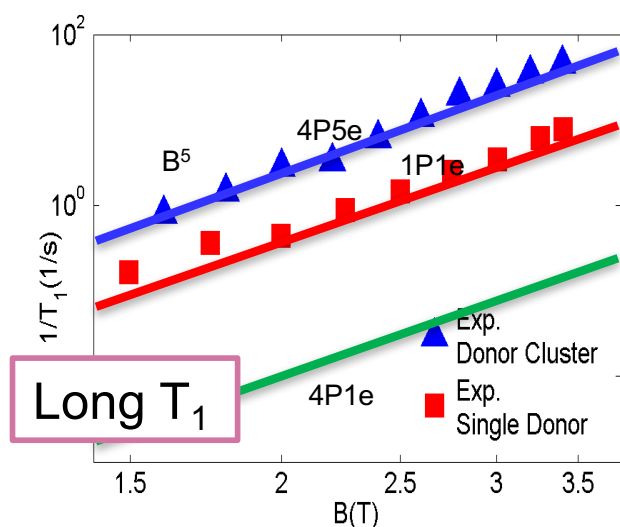
- J increases \rightarrow energy gap increases \rightarrow more phonon can couple \rightarrow shorter T_1
- $H = \begin{pmatrix} -3J & A \\ A & J \end{pmatrix}$ Mixing $\sim A/J \rightarrow$ larger J , smaller mixing, longer T_1

Singlet-triplet T_1 decreases with J , increases with R

- An accurate method: FCI+TB to treat $2e T_1$
- Close match to experiment value.



- By developing a method to treat the one-electron to multi-electron spin-relaxation problems and understanding the mechanisms behind, it is easier to design a quantum computer with high-fidelity using donors in Si nanoelectronic devices.



- Prof. Rajib Rahman, Prof. Gerhard Klimeck, Prof. Michelle Simmons, Prof. Lloyd Hollenberg, Prof. Supriyo Datta, Prof. Zhihong Chen, Dr. Bent Weber, Dr. Thomas Watson and Dr. Jim Fonseca
- Yaohua Tan, Archana Tankasala, Rifat Ferdous, Yu Wang, Harshad Sahasrabudhe, Chin-Yi Chen, Hesam Ilatikhameneh, Tarek Ameen, Kuang-Chung Wang, Prasad Sarangapani, Junzhe Geng, Zhengping Jiang, Kai Miao, Yu He, Fabio Chu, Xufeng Wang, Pengyu Long, Fan Chen, Daniel Mejia, Saumitra Mehrotra, Jun Huang, Bozidar Novakovic, Matthias Tan, Parijat Sengupta, Mehdi Salmani and Ganesh Hedge.
- Thanks to all other friends.

Thank You

- Part I: The tight-binding $T_1 \rightarrow$ Y. L. Hsueh et al., Phys. Rev. Lett. 113, 246406 (2014)
- Part II: T_1 in devices with electric fields \rightarrow B. Weber et. al., “A Single-Atom Probe of the Silicon Qubit Environment” (submitted)
- Part III: Two electron T_1 problem \rightarrow Drafted

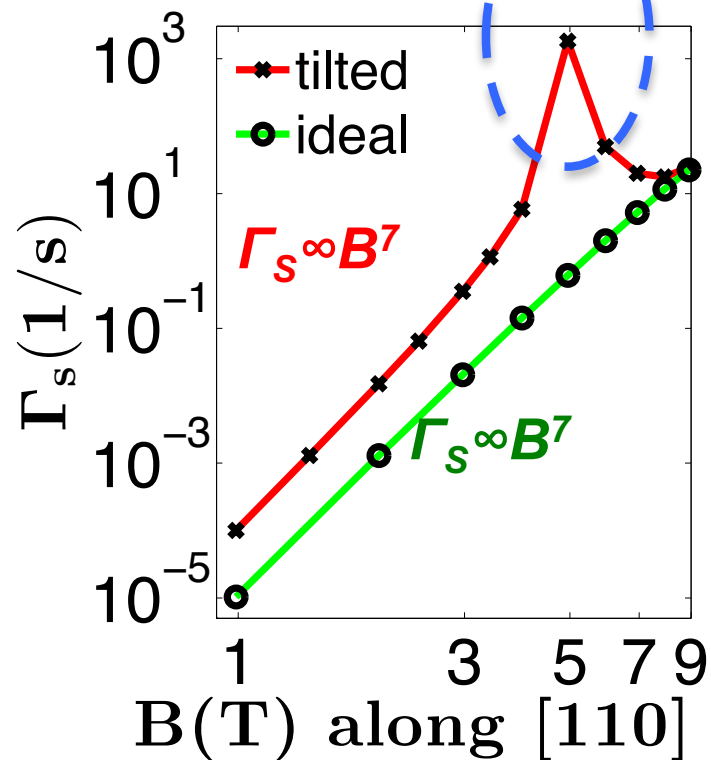
$$\begin{aligned}\hat{U}_{ij} = & \frac{1}{2} \sum_q \left(\frac{\hbar}{2V\rho\omega_q} \right)^{(1/2)} i(e_{qi}q_j + e_{qj}q_i) \{ \hat{a}_q^+ \exp[i(\mathbf{q} \cdot \mathbf{r})] \\ & + \hat{a}_q \exp[-i(\mathbf{q} \cdot \mathbf{r})] \},\end{aligned}\quad (4)$$

where V is the volume of the crystal, ρ the mass density, and \mathbf{e}_q the phonon polarization unit vector. Using Eqs. 2 and 4, the matrix element of \hat{H}_{ep} can be expressed as,

$$\begin{aligned}\langle n', n_q + 1 | \hat{H}_{ep} | n, n_q \rangle \\ = \frac{1}{2} \sum_q \left(\frac{\hbar}{2V\rho\omega_q} \right)^{(1/2)} \sqrt{n_q + 1} \\ \times \sum_{i,j} i(e_{qi}q_j + e_{qj}q_i) \langle n' | \exp[i(\mathbf{q} \cdot \mathbf{r})] \hat{\Xi}_{ij} | n \rangle.\end{aligned}\quad (5)$$

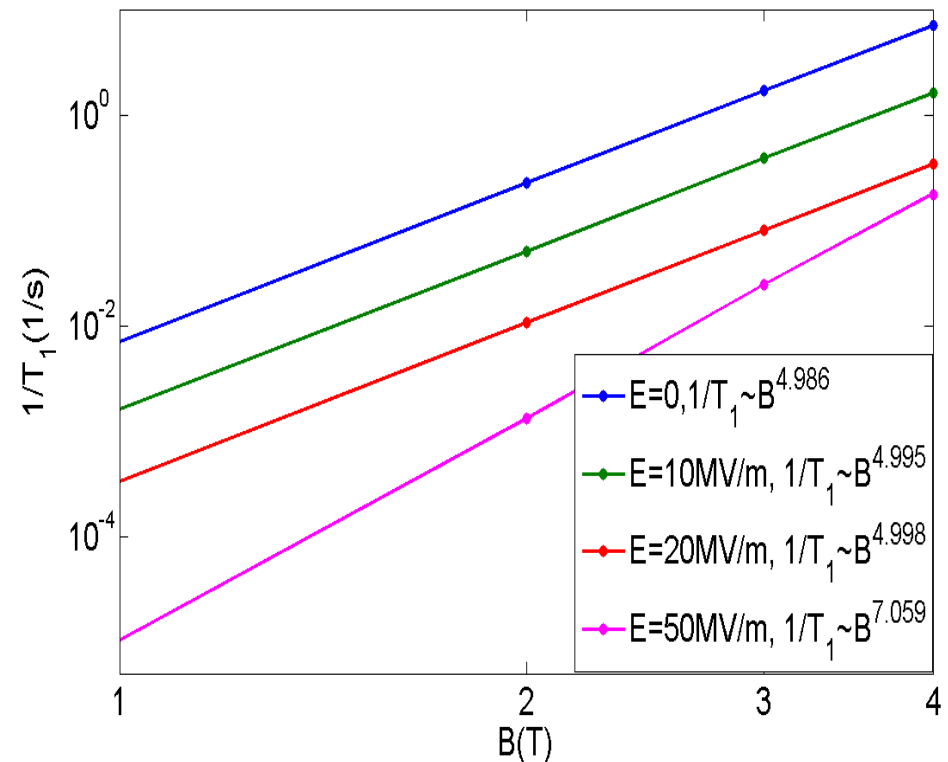
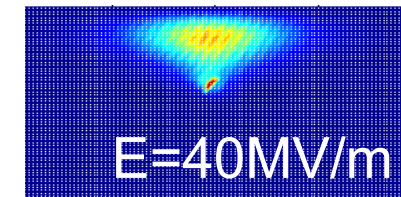
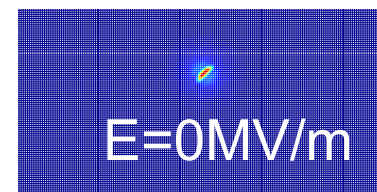
Quantum Dots

Relaxation hot-spot at $E_{zs}=E_{vs}$

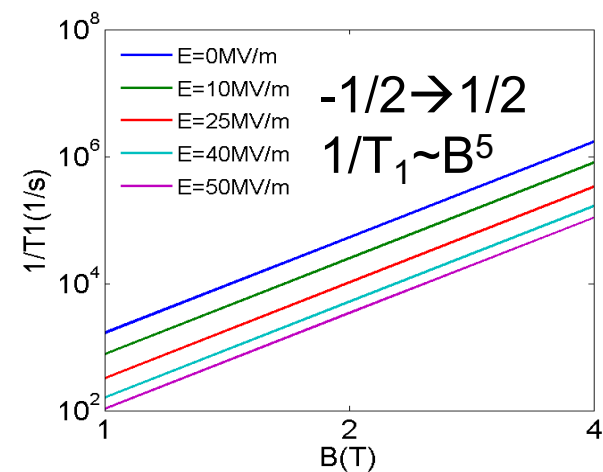
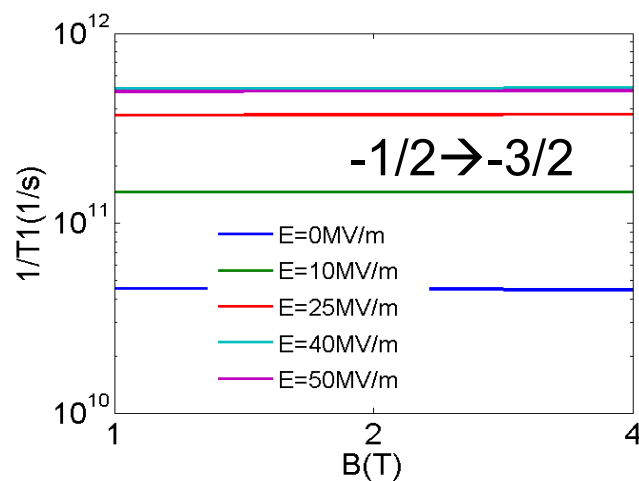
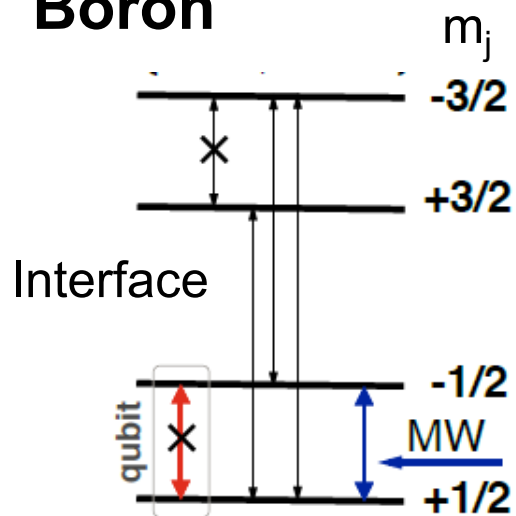


Rifat Ferdous

Interface donor

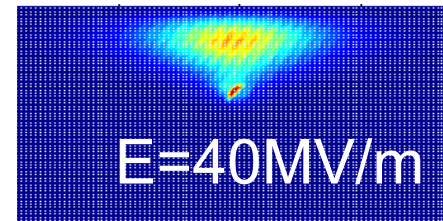
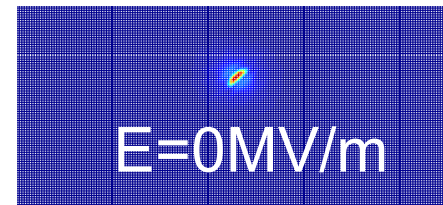
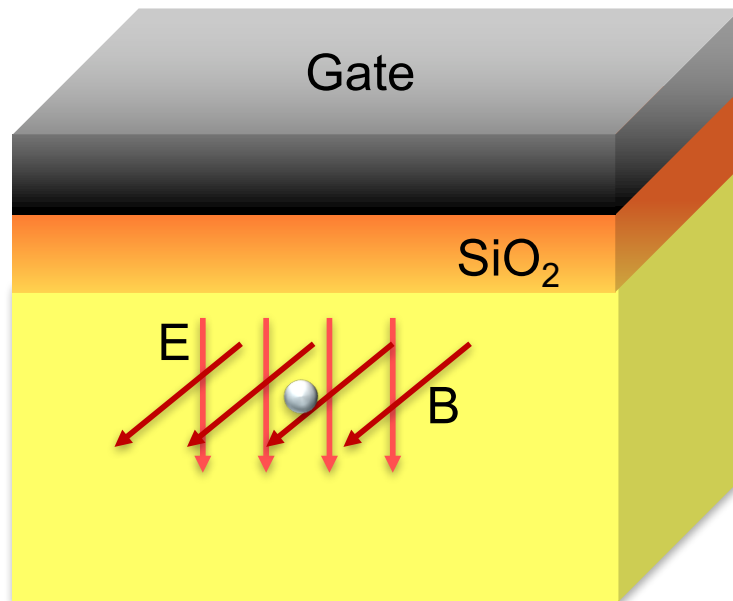


Boron



Motivation

- Hybridized donor states has been investigated both experimentally and theoretically.
- Lack of comprehensive study of T_1 times in these hybridized system.

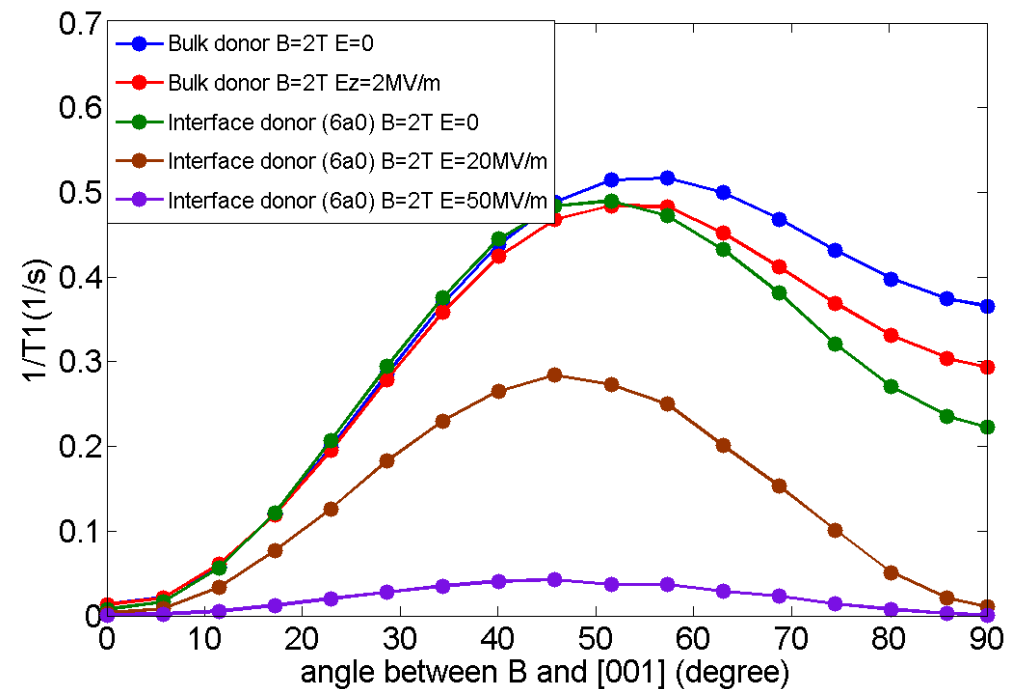
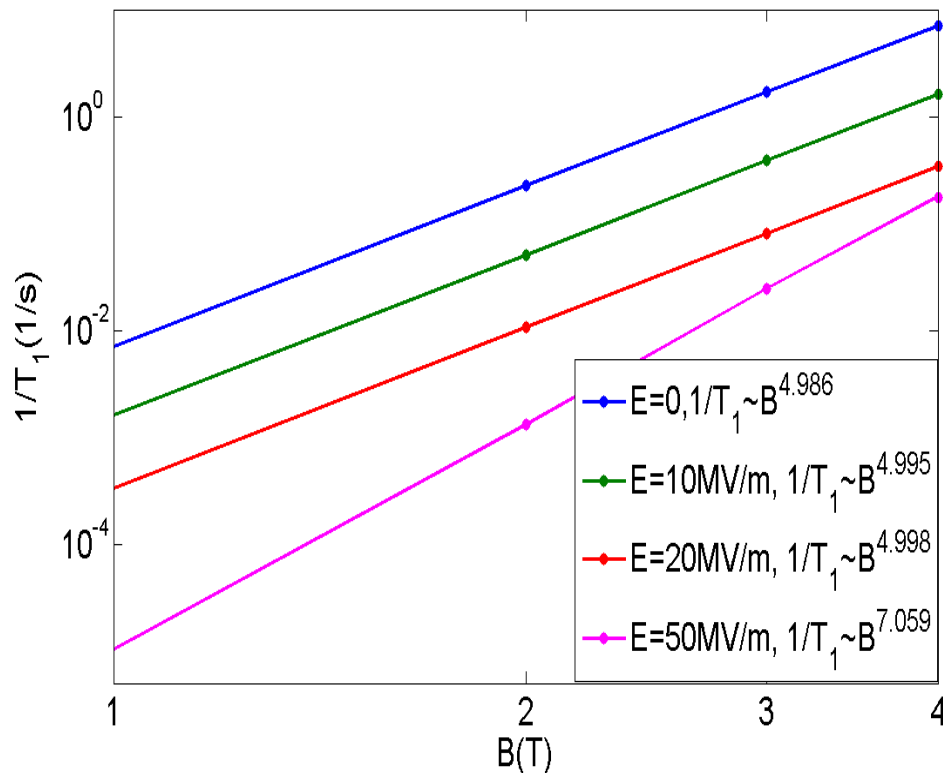


Method

- Interface donor states obtained from full-band tight-binding approach.
- Atomistic T_1 calculation.

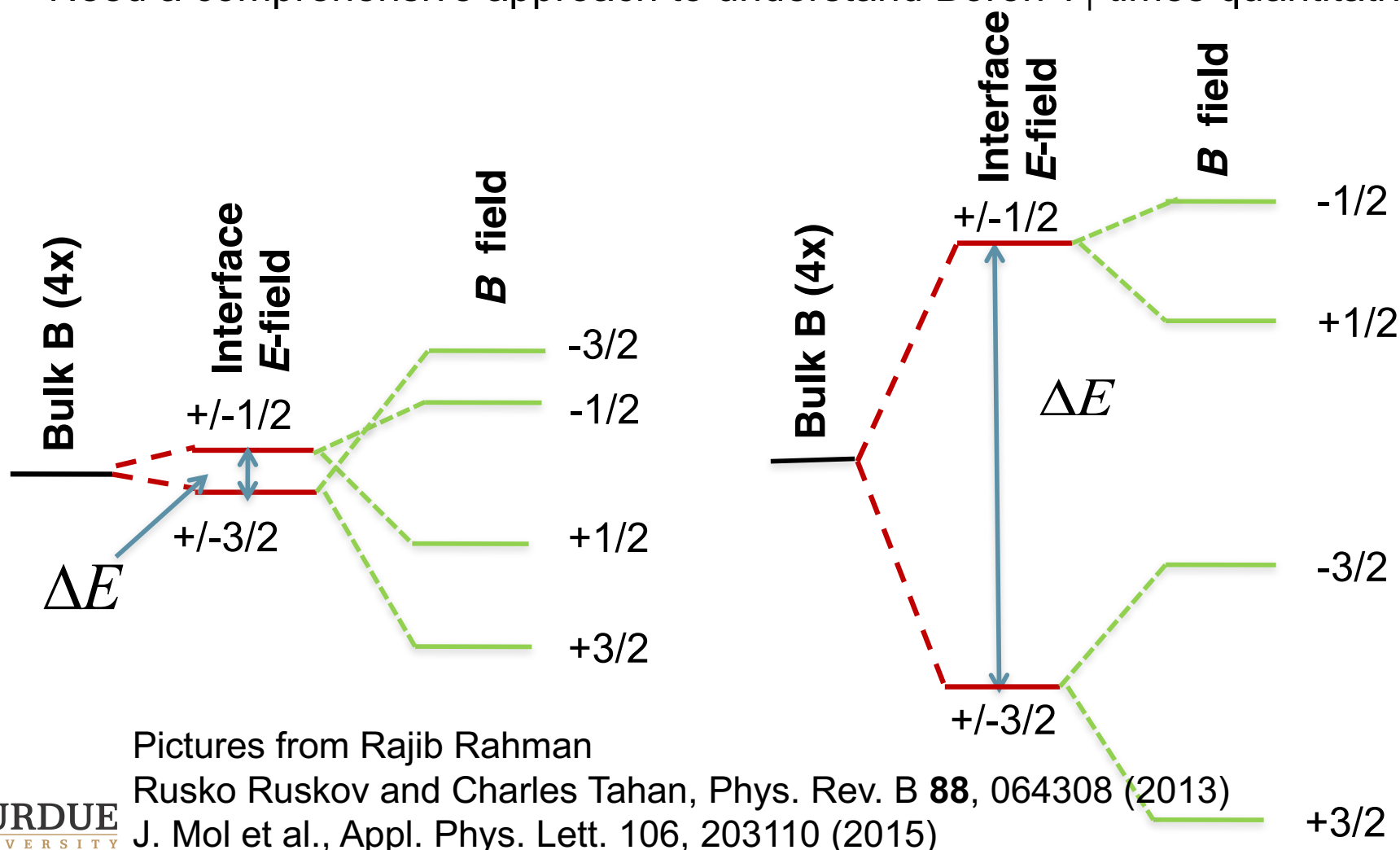
Results

- $1/T_1 \sim B^5$ to B^7 transition as electron states move to the interface.
- T_1 anisotropy change with symmetry/valley information.



Motivation

- Qubit proposal using Boron acceptor has attracted some interest.
- T_1 mechanism in Boron has been studied theoretically.
- Need a comprehensive approach to understand Boron T_1 times quantitatively.



Pictures from Rajib Rahman

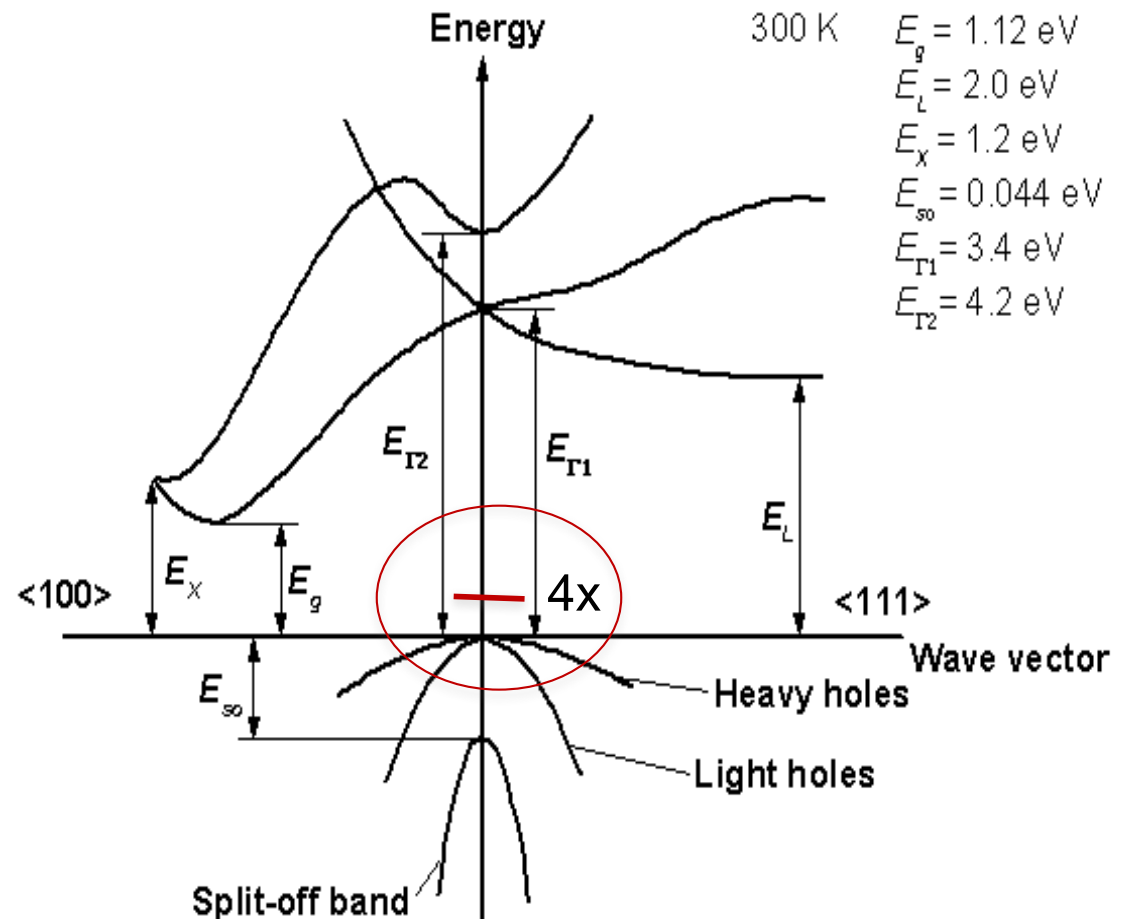
Rusko Ruskov and Charles Tahan, Phys. Rev. B **88**, 064308 (2013)

J. Mol et al., Appl. Phys. Lett. 106, 203110 (2015)

Method

- Bulk Boron and interface Boron states obtained from full-band tight-binding approach.
- Atomistic T_1 calculation.

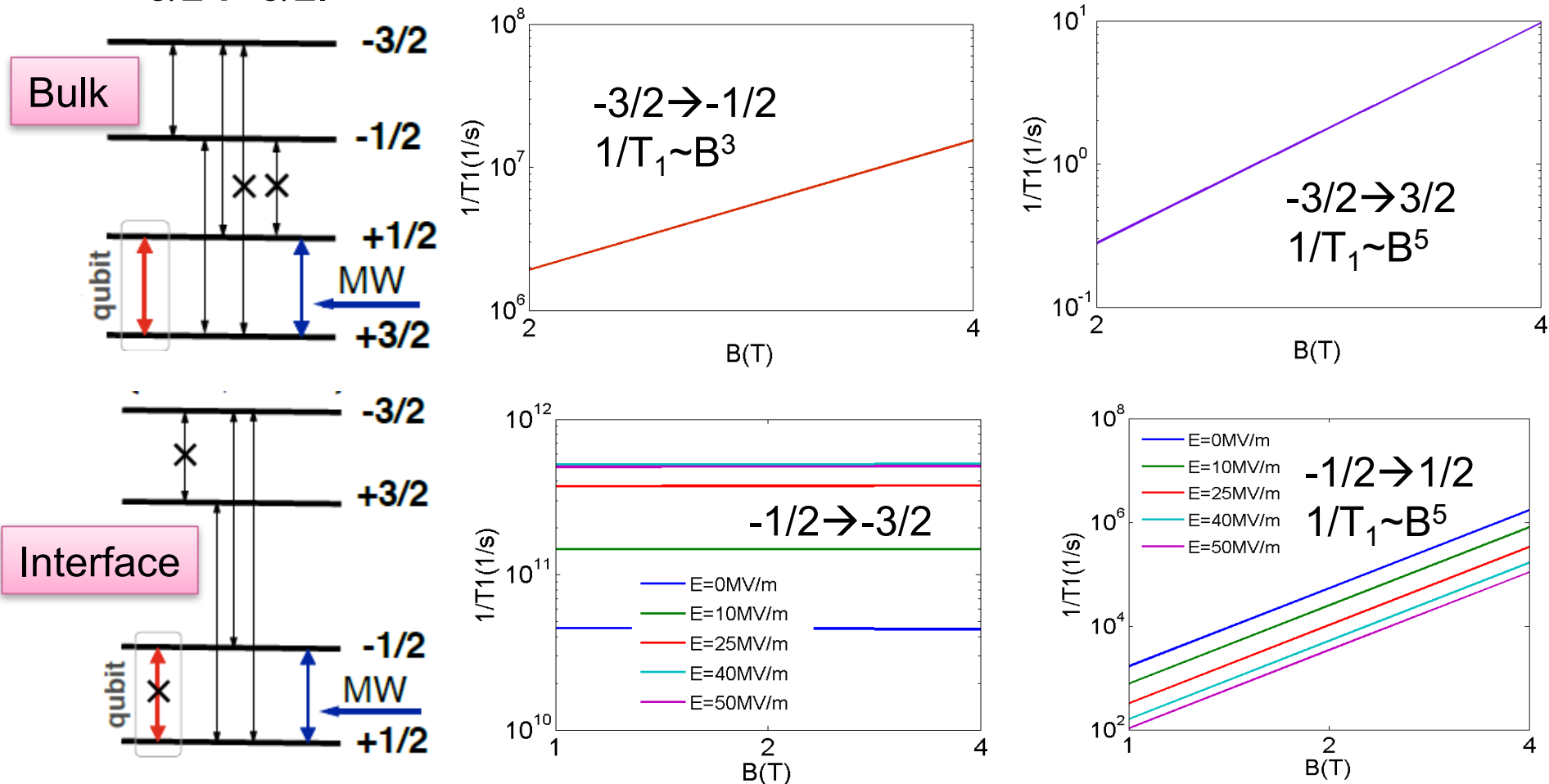
Ground state of Boron at 45 meV above VB



Si Bandstructure

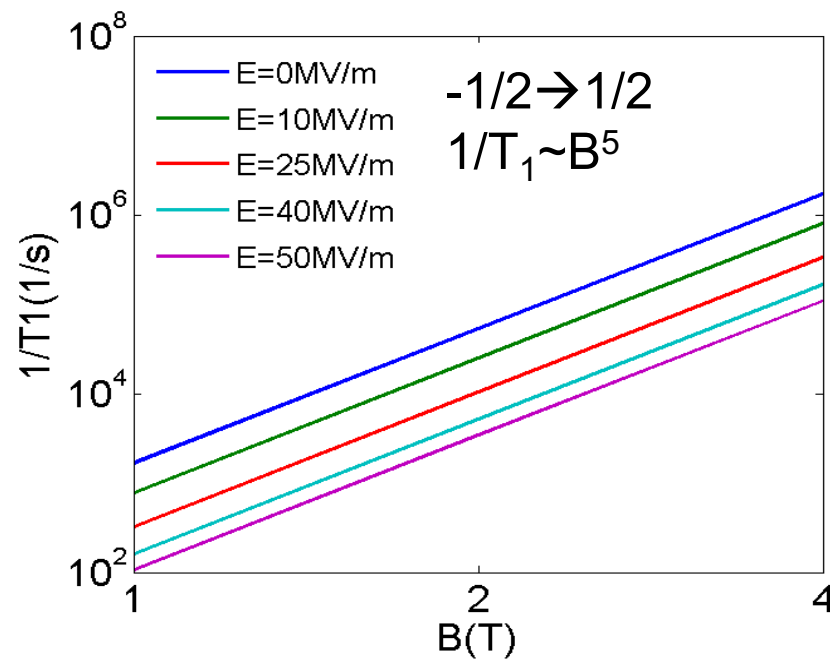
Preliminary Results

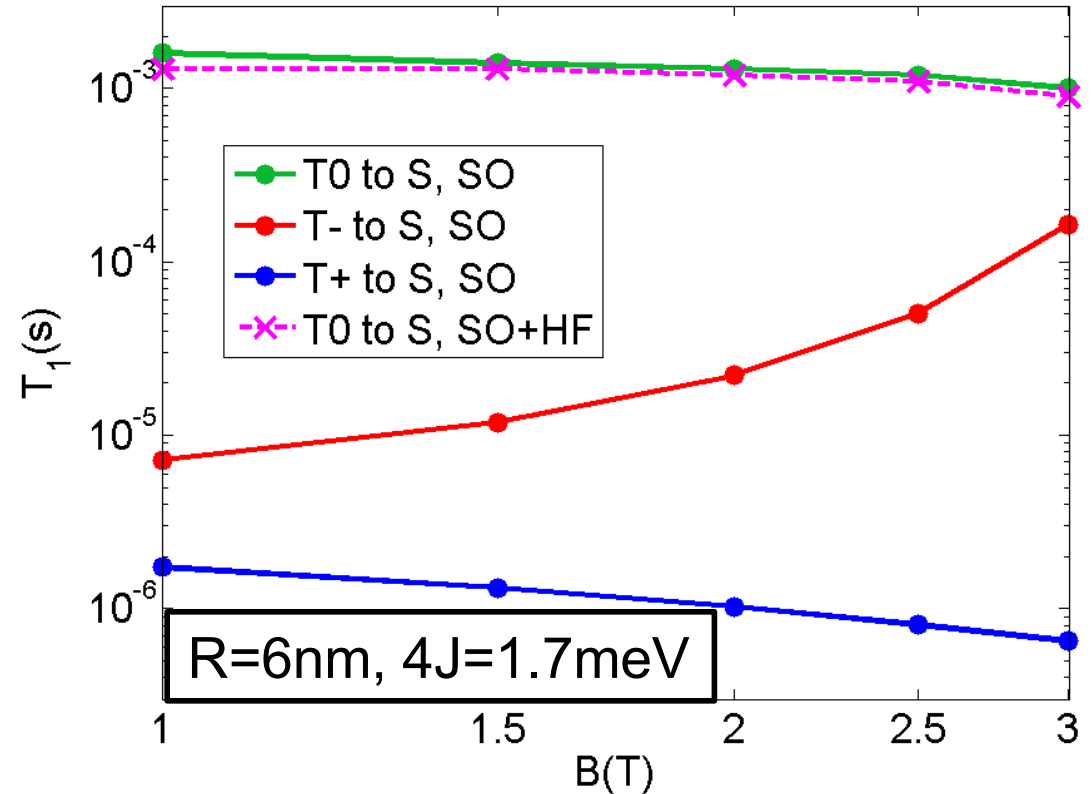
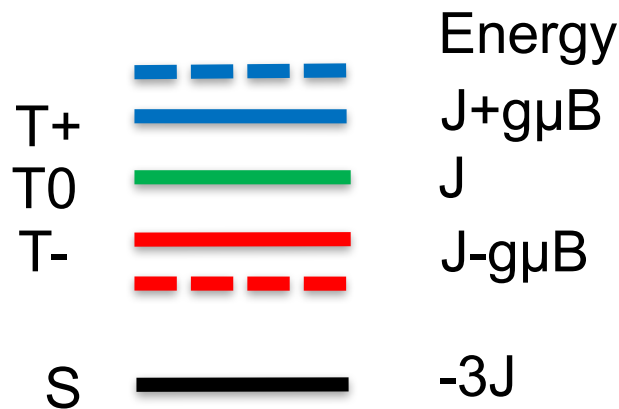
- Bulk Boron: $1/T_1 \sim B^3$ for $\pm 1/2 \rightarrow \pm 3/2$, $1/T_1 \sim B^5$ for $+1/2 \rightarrow -1/2$ and $+3/2 \rightarrow -3/2$
- Interface Boron: No B dependency for $\pm 1/2 \rightarrow \pm 3/2$, $1/T_1 \sim B^5$ for $+1/2 \rightarrow -1/2$ and $+3/2 \rightarrow -3/2$.



Expected Results

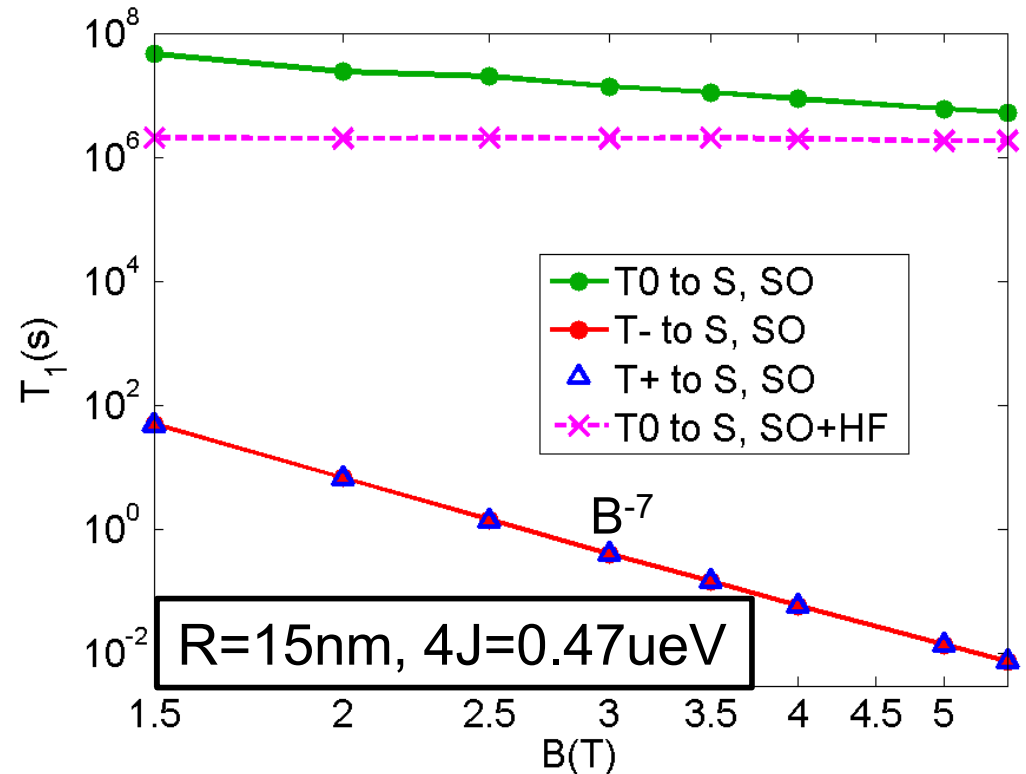
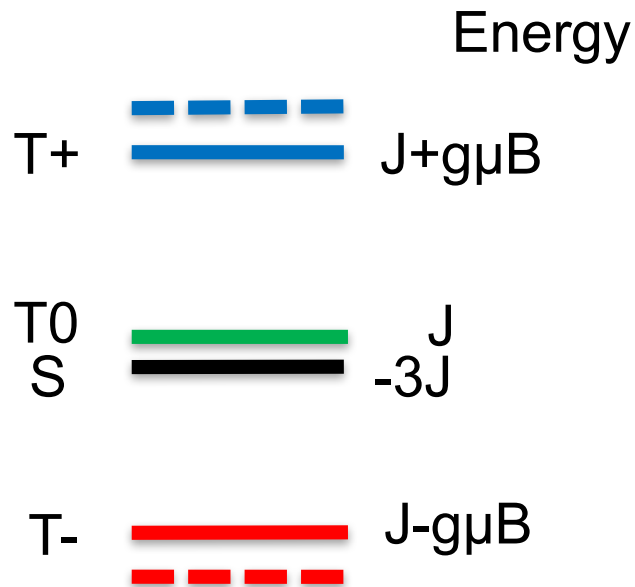
- Explain the $1/T_1$ magnitude and B dependencies in both bulk and interface Boron.
- Explain the T_1 magnitude change with electric field for Boron near interface.





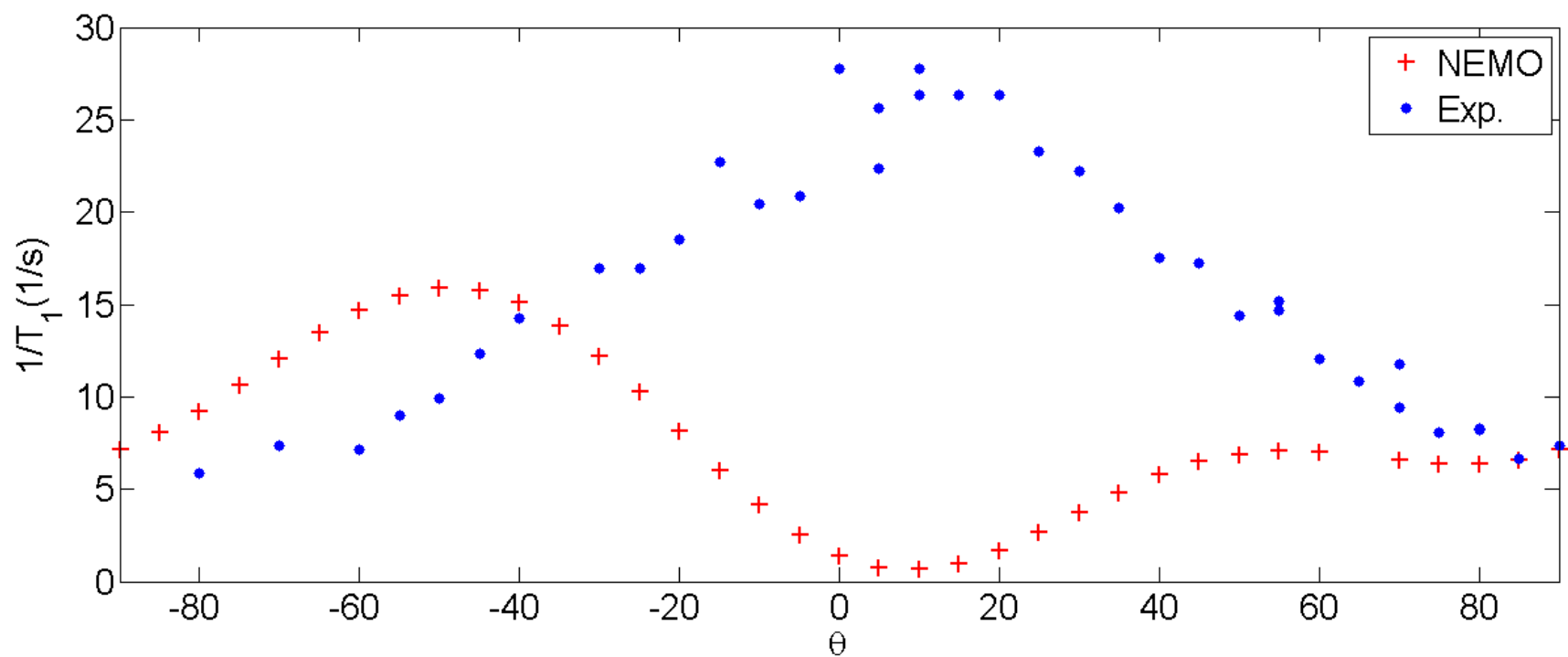
- As energy gap increases \rightarrow more phonon can couple \rightarrow shorter T_1
- Weak B dependence
- SO dominates ($A/J \sim 0$)

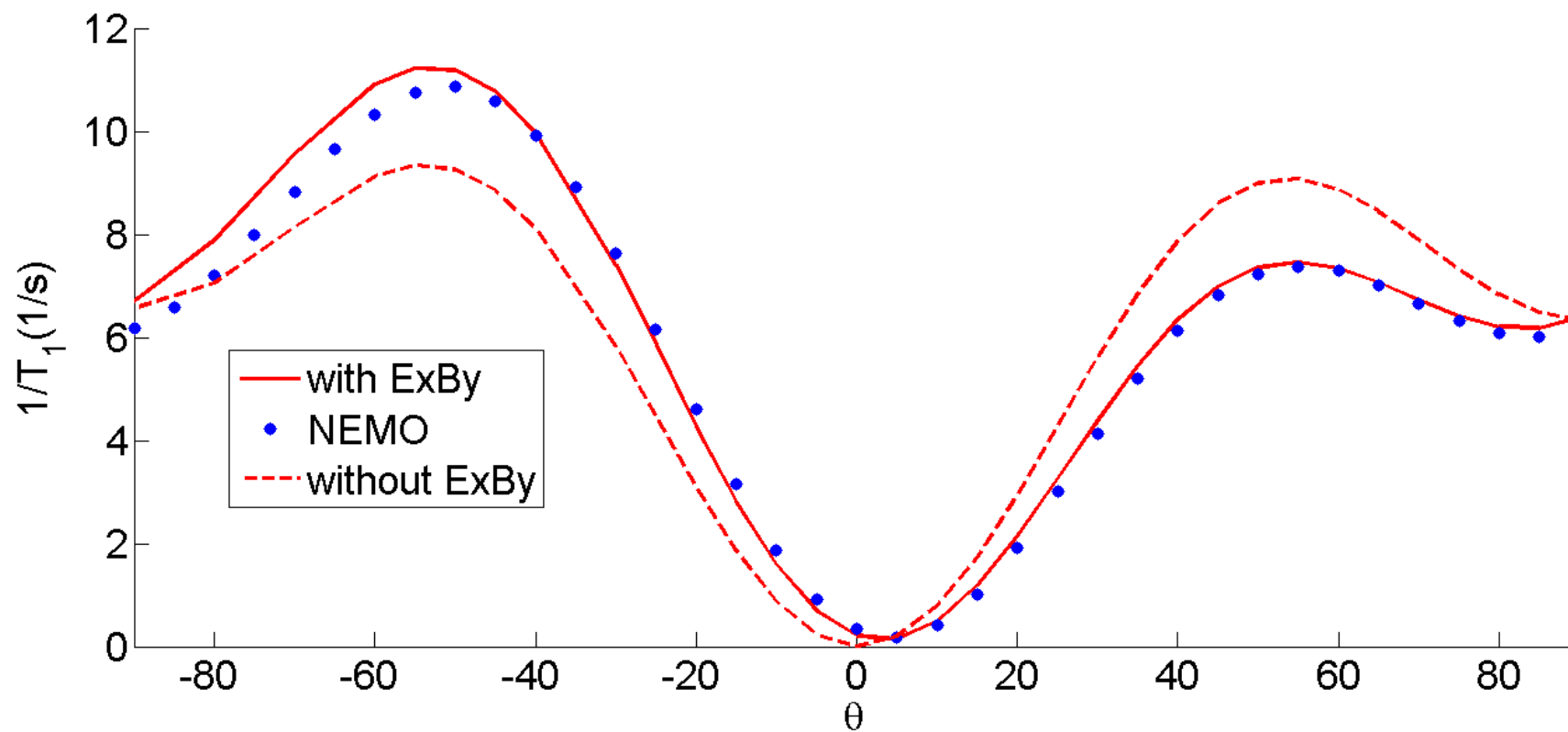
For $R=6\text{nm}$, weak B dependence, SO dominates.



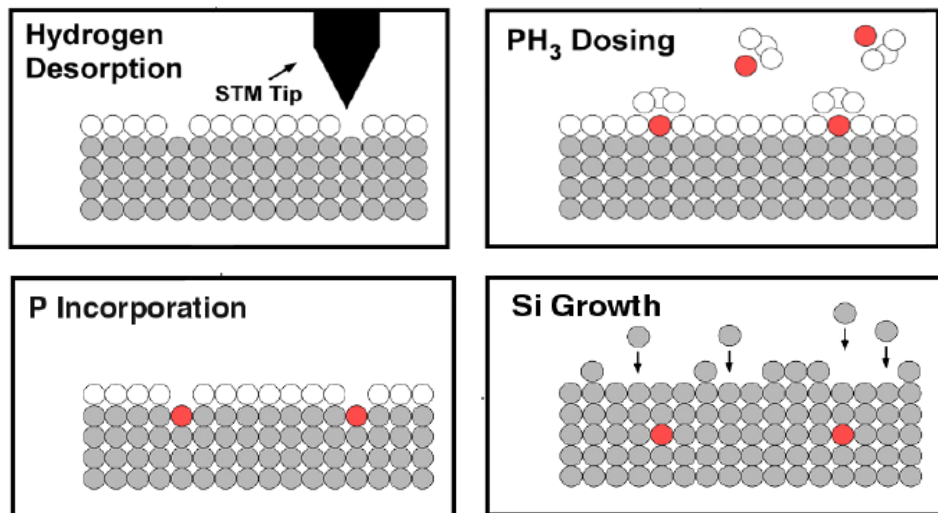
- As energy gap increases \rightarrow more phonon can couple \rightarrow shorter T_1
- Strong B dependence
- Hyperfine dominates (A/J large)

For $R=15\text{nm}$, strong B dependence, hyperfine dominates.

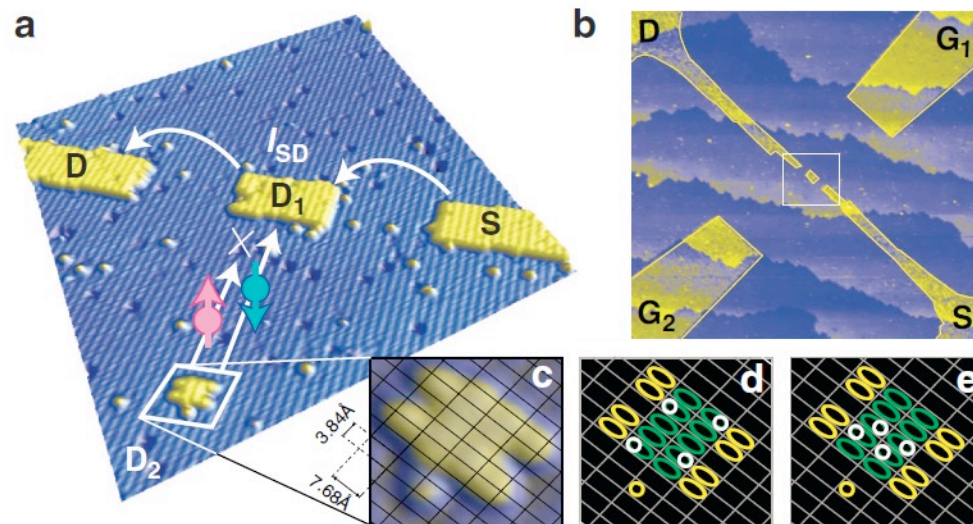
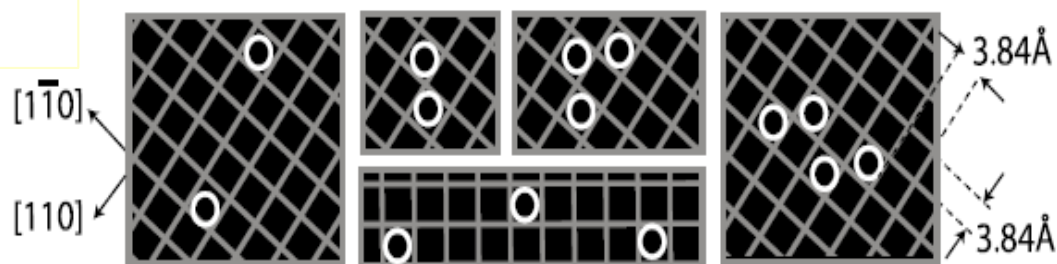




Place donor with atomic precision



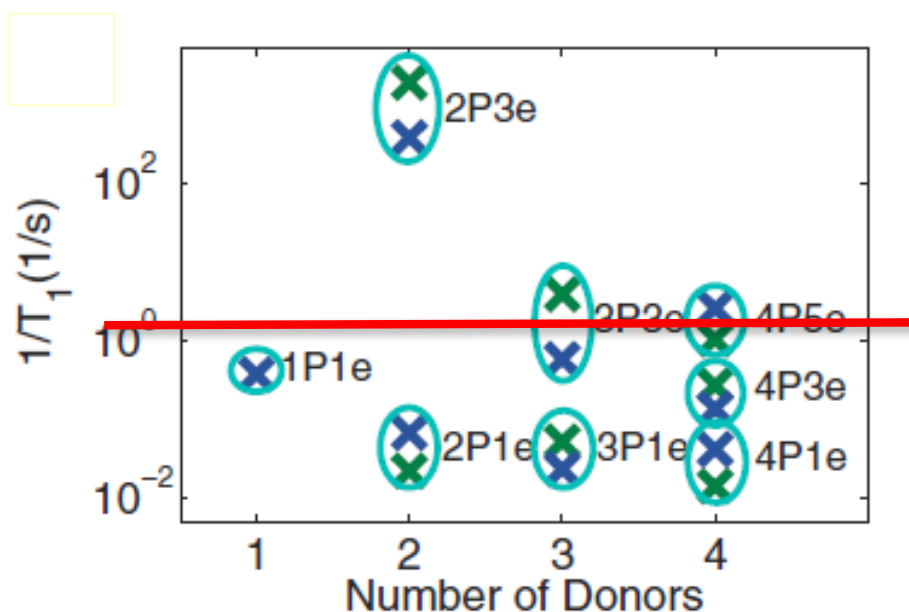
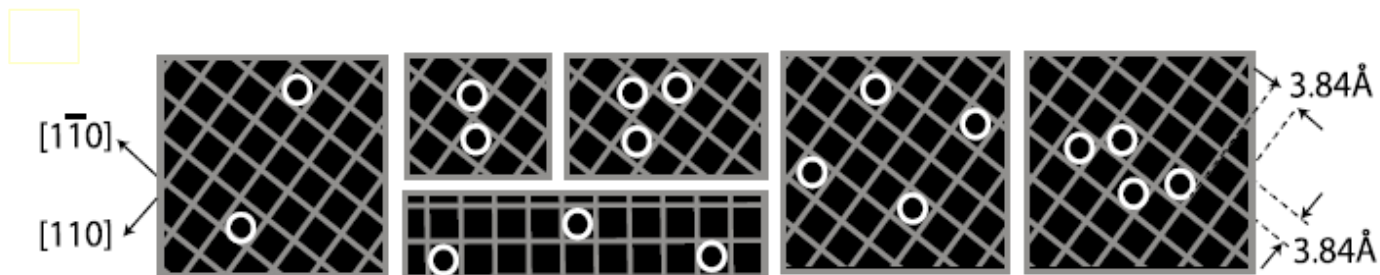
Donor Cluster



H. Büch et al. Nature Communications 4, 2017 (2013)

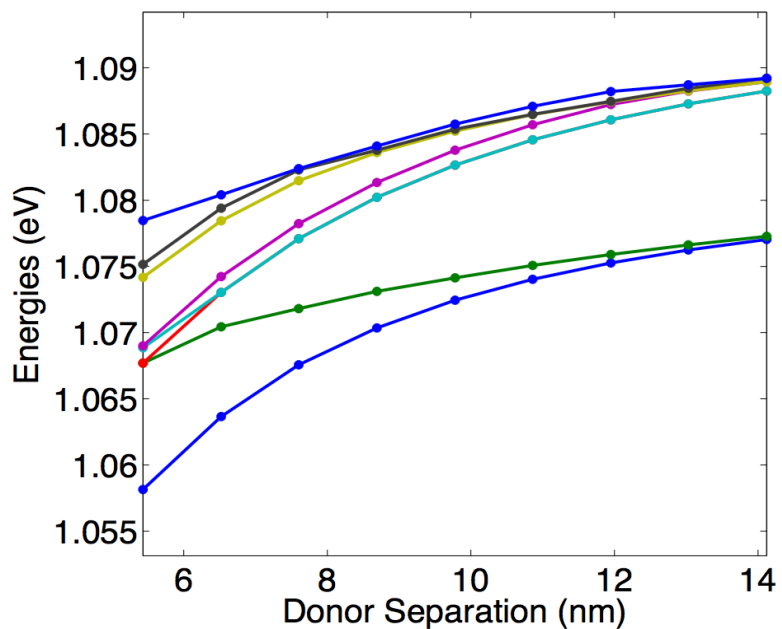
Unknown:
Donor/electron number

The exact donor/electron number in a donor cluster is unknown.

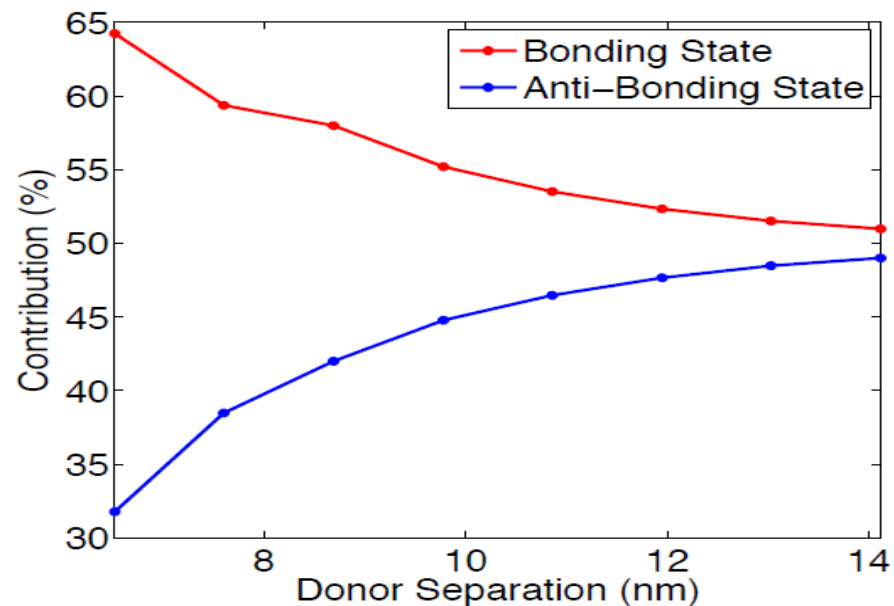


Measuring T_1 can serve as a non-invasive method to help determine the donor/electron number in the donor cluster.

Single Electron Energies



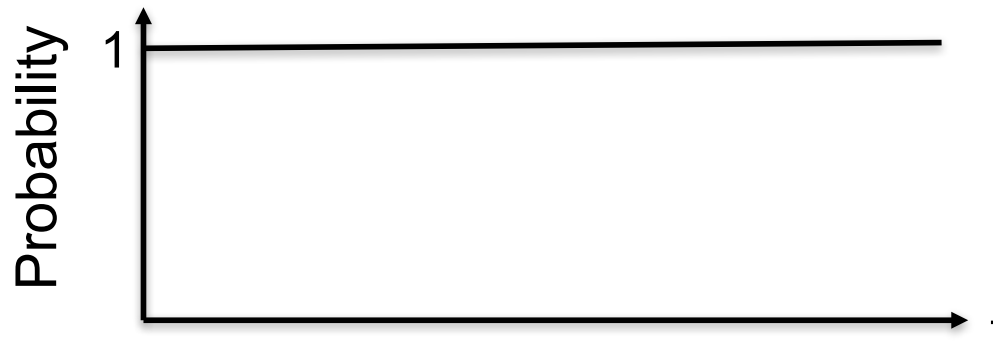
[100] Donor Separation; Bulk Donor Depth
CI GS Contributions



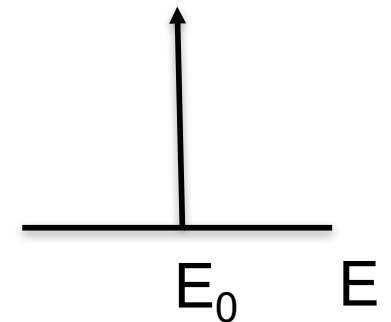
$$\text{Hep}(r_1, r_2) = \text{Hep}(r_1) + \text{Hep}(r_2)$$

● $|\uparrow\rangle$ Stationary states

— $|\downarrow\rangle$

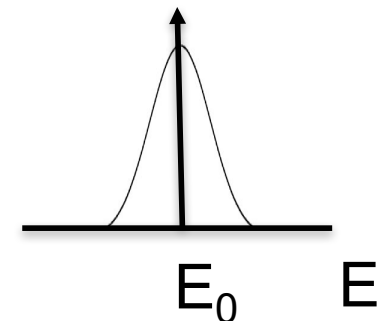
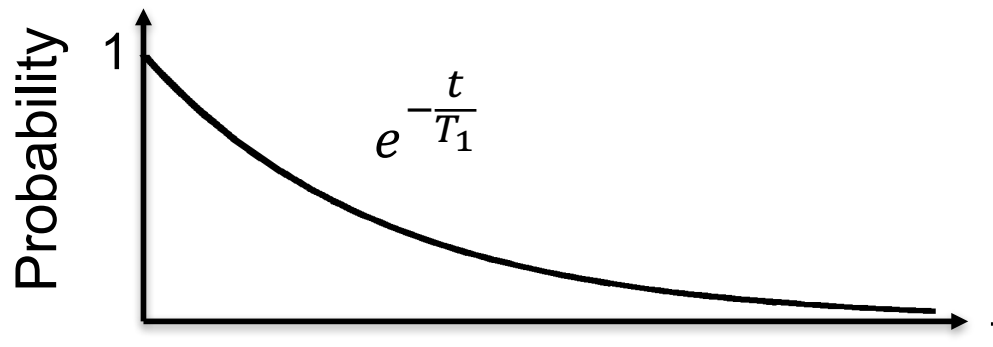


Energy spectrum



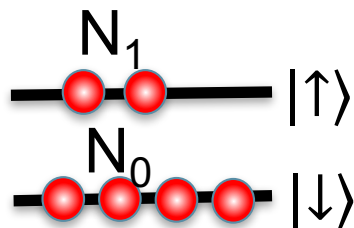
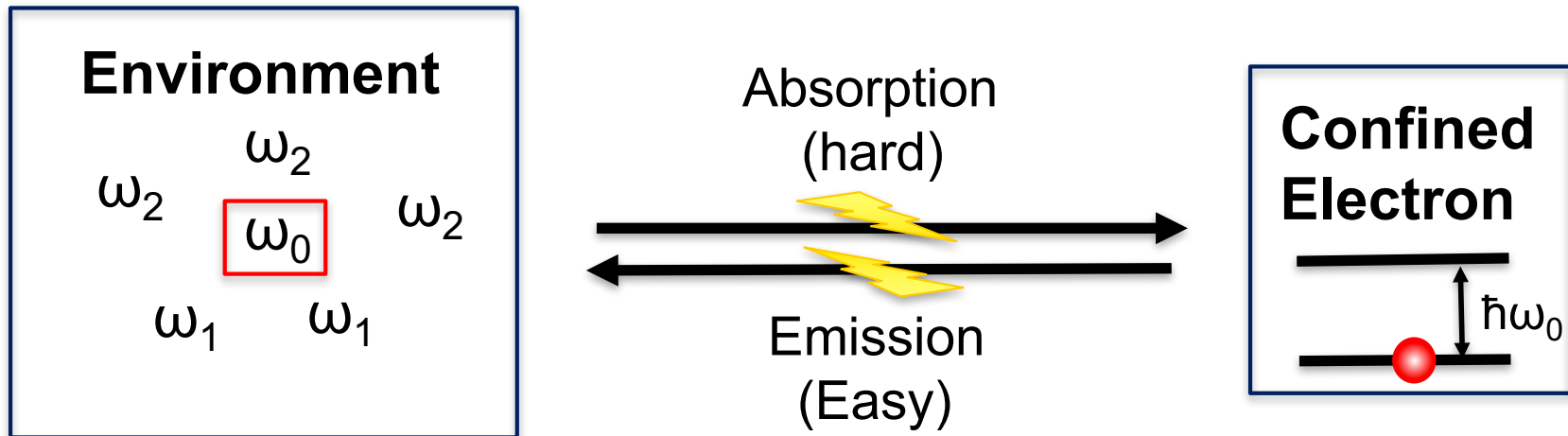
● $|\uparrow\rangle$ States with finite lifetime

— $|\downarrow\rangle$



Scattering processes result in finite lifetime of electron states and energy broadening.

Why does the electron want to be at its lower energy state?

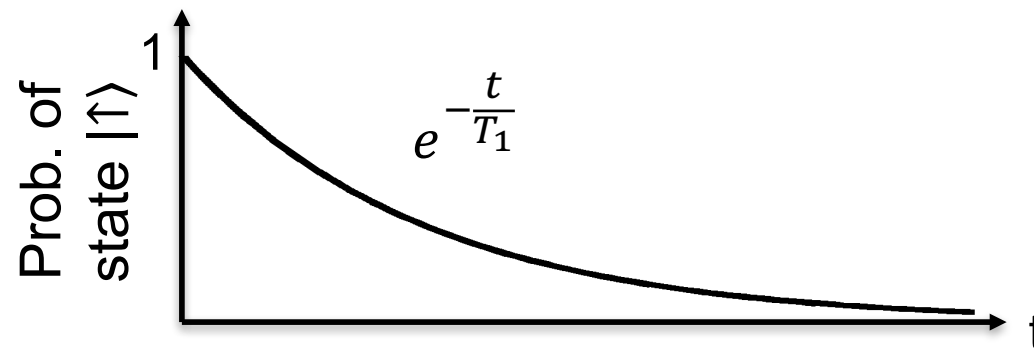
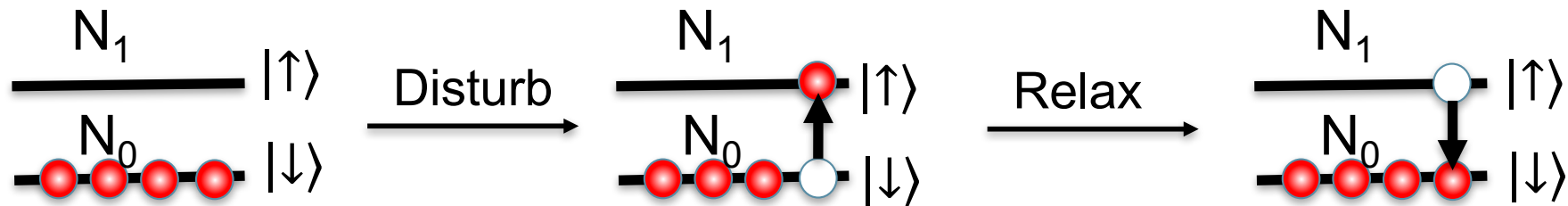


$$N_0 \times (\text{Absorption rate}) = N_1 \times (\text{Emission rate})$$

large small small large

Emission rate is always greater than absorption rate at thermal equilibrium $\rightarrow N_0 > N_1$

At low temperature ($<2\text{K}$)



The T_1 time is the characteristic time to restore the system to thermal equilibrium

$$H_{SO}^{eff} = \underbrace{R(\mathbf{k} \times \mathbf{E})}_{\mathbf{B}^{eff}} \cdot \begin{pmatrix} \alpha_X & & \\ & \alpha_Y & \\ & & \alpha_Z \end{pmatrix} \cdot \boldsymbol{\sigma}$$