

Engineering Multi-Electron Interactions for Quantum Logic in Silicon

PHD FINAL EXAMINATION

Archana Tankasala

Electrical and Computer Engineering
Purdue University USA

Electron Spin Qubits in Solid-State Architectures

Modeling via Atomistic Configuration Interaction

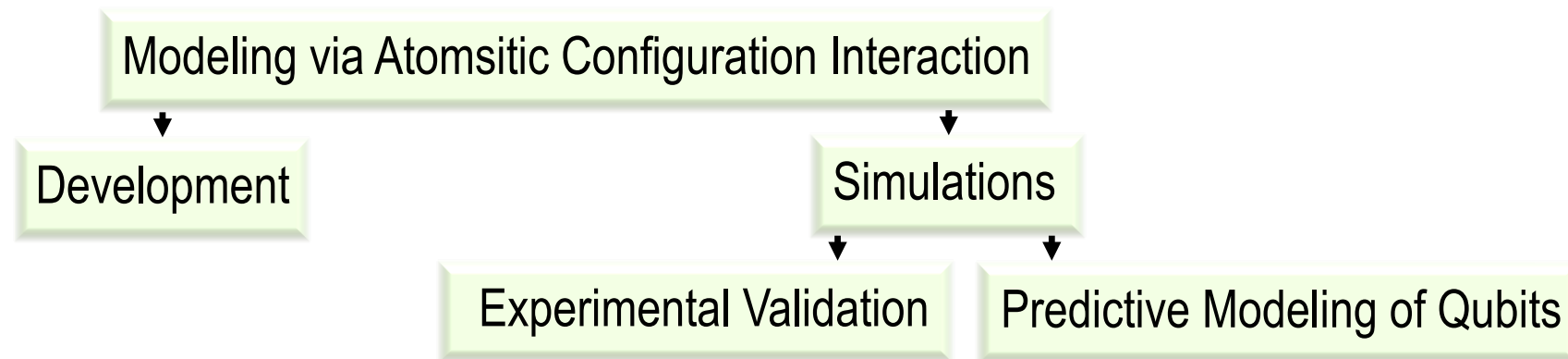
Development

Simulations

Experimental Validation

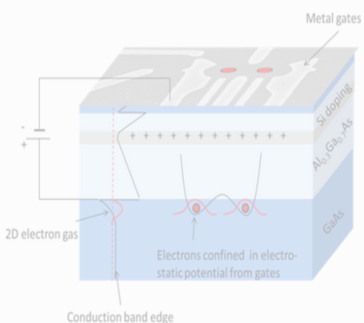
Predictive Modeling of Qubits

Electron Spin Qubits in Solid-State Architectures

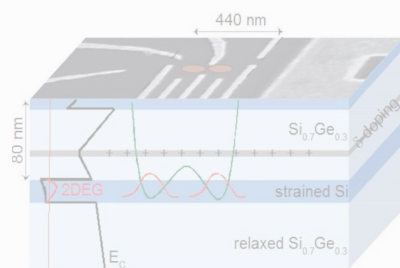


- ✓ Advantages with fabrication technologies of modern electronics

GaAs-AlGaAs



Si-SiGe



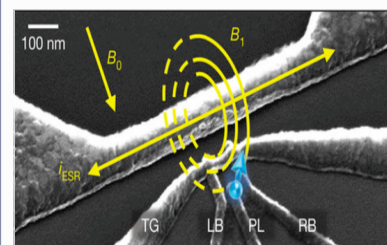
Si MOS



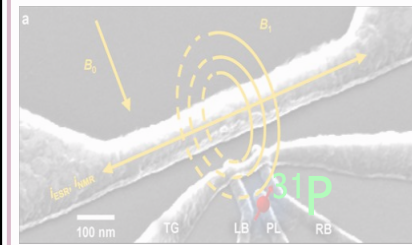
Electron Spin Qubit

Electrostatic Gate Confinement

Si: P



Si: P



Nuclear Spin Qubit

Coulombic Donor Confinement

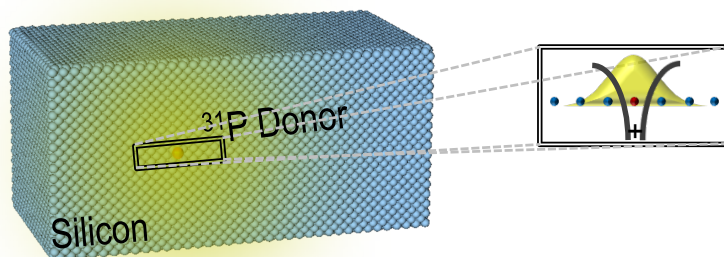
Electron spin qubits bound to dopant atoms in silicon

^{1,3}<http://www.accent.rwth-aachen.de/>

²Lai, N. S., et al. Scientific reports (2011)

⁴Pla, Jarryd J., et al. Nature 489.7417 (2012)

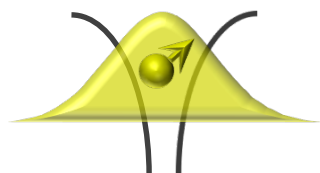
Single electron spin qubits bound to dopant atoms in silicon



Coulombic potential

➤ Spherically symmetric

Confines electron in 3D



✓ Single electron spin qubit demonstrated successfully

LETTER

doi:10.1038/nature11449

A single-atom electron spin qubit in silicon

Jarryd J. Pla¹, Kuan Y. Tan¹†, Juan P. Dehollain¹, Wee H. Lim¹, John J. L. Morton²†, David N. Jamieson³, Andrew S. Dzurak¹ & Andrea Morello¹

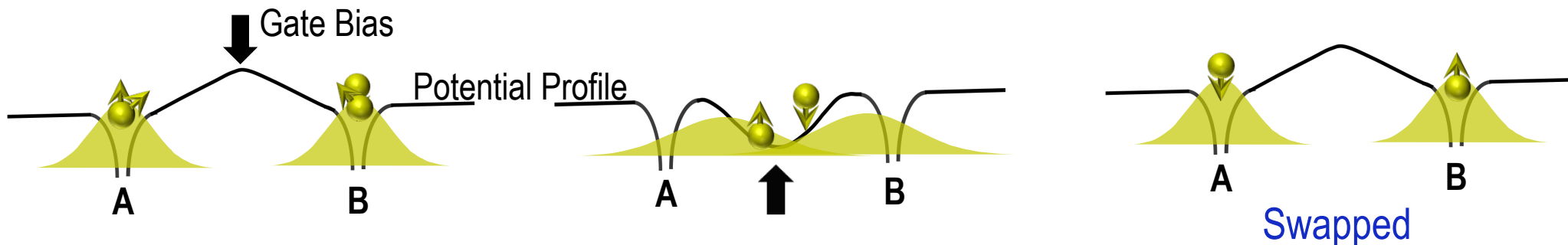
LETTER

doi:10.1038/nature09392

Single-shot readout of an electron spin in silicon

Andrea Morello¹, Jarryd J. Pla¹, Floris A. Zwanenburg¹, Kok W. Chan¹, Kuan Y. Tan¹, Hans Huebl¹†, Mikko Möttönen^{1,3,4}, Christopher D. Nugroho¹†, Changyi Yang², Jessica A. van Donkelaar², Andrew D. C. Alves², David N. Jamieson², Christopher C. Escott¹, Lloyd C. L. Hollenberg², Robert G. Clark¹† & Andrew S. Dzurak¹

Two qubit gates are the next big challenge for quantum computing applications

Example: **SWAP** Operation

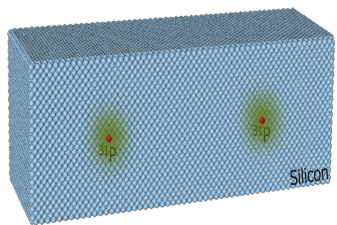
Electron spins rotate in presence of each other

When to stop applying the gate bias?

➤ Speed of electron spin rotation → **Electron-Electron Interaction**

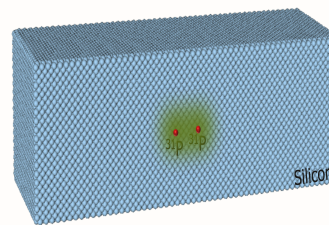
✓ Two Qubit operations rely on interaction strength between two electrons

Electron-Electron Interactions must be accurately estimated for precise qubit control



Heitler-London Approximation

✓ Well separated donors

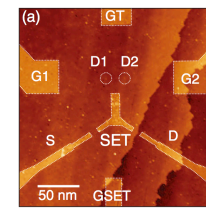
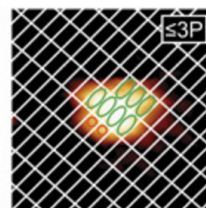
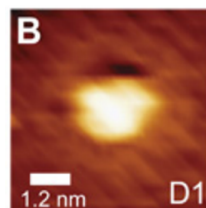


Hartree-Fock Approximation

✓ Closely spaced donors

Realistic Quantum Computing Devices

Donor separations range from 1nm (donor clusters) to 25nm (spin qubit)

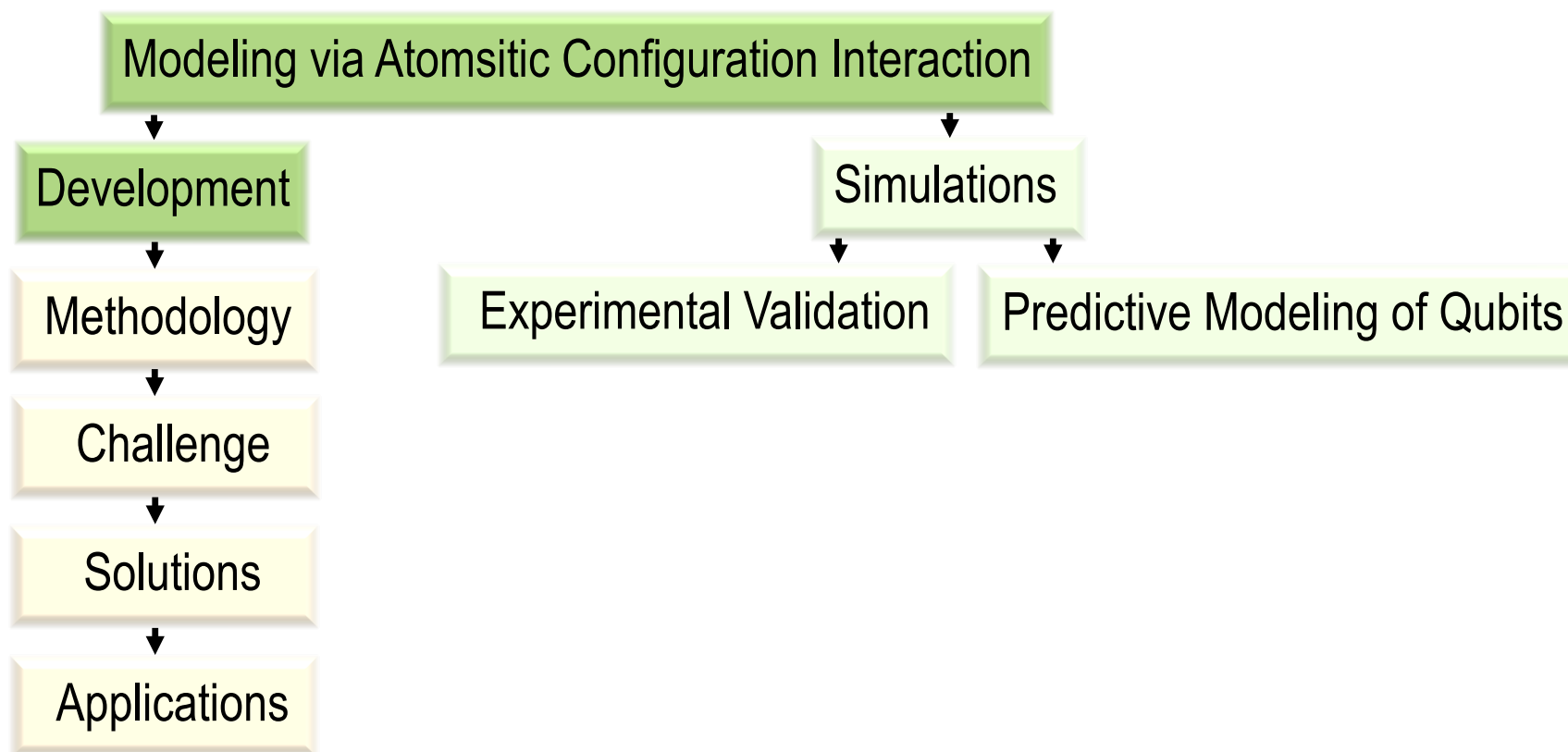


Exact electron-electron interactions for precise qubit control

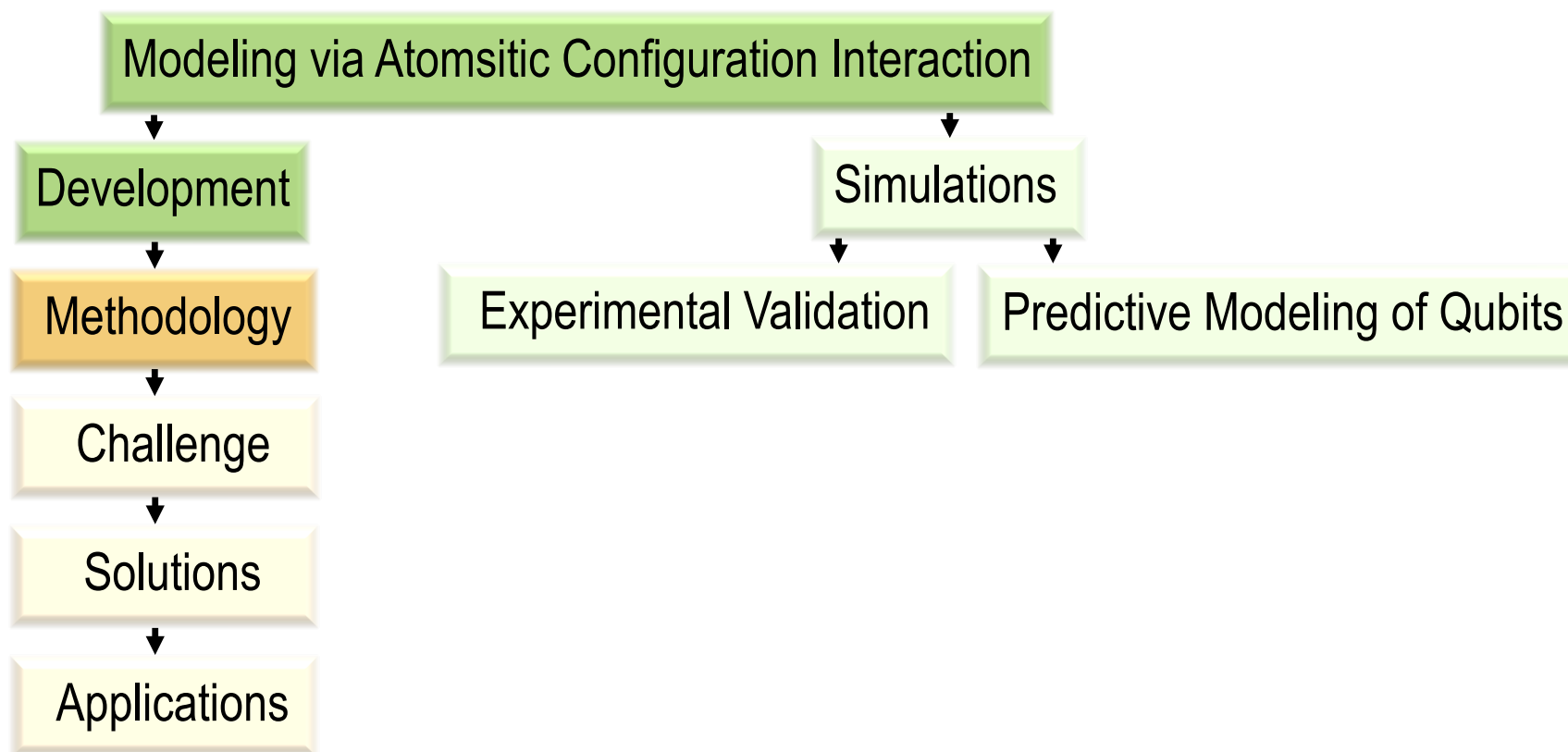
GOAL

Model to capture electron-electron interactions **accurately** for **ALL** donor separations

Electron Spin Qubits in Solid-State Architectures



Electron Spin Qubits in Solid-State Architectures



ALL electron-electron interactions

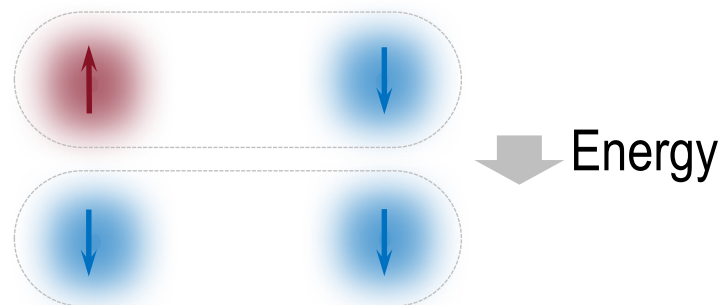
- ✓ Coulomb repulsion

Electron **charge** clouds



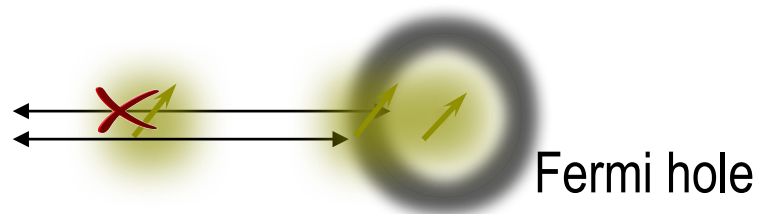
- ✓ Exchange interactions

Parallel electron **spins** (Hund's Rule)



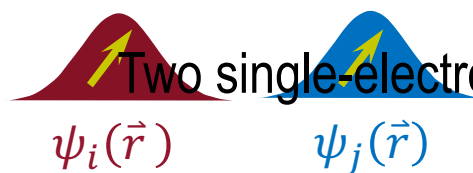
- ✓ Correlations

Correct overestimated repulsion

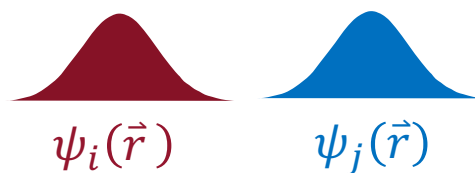


Full Configuration Interaction (FCI) to model electron-electron interactions

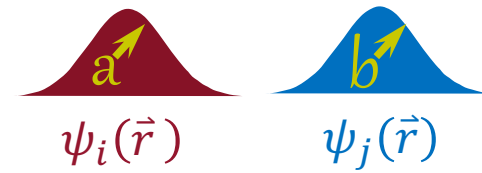
Two single-electron states:



$\psi_i(\vec{r})$ $\psi_j(\vec{r})$



$\psi_i(\vec{r})$ $\psi_j(\vec{r})$



$\psi_i(\vec{r})$ $\psi_j(\vec{r})$

Two electrons:

$$\Psi_{ij}(\vec{r}_a, \vec{r}_b) = \psi_i(\vec{r}_a) \psi_j(\vec{r}_b) - \psi_i(\vec{r}_b) \psi_j(\vec{r}_a)$$

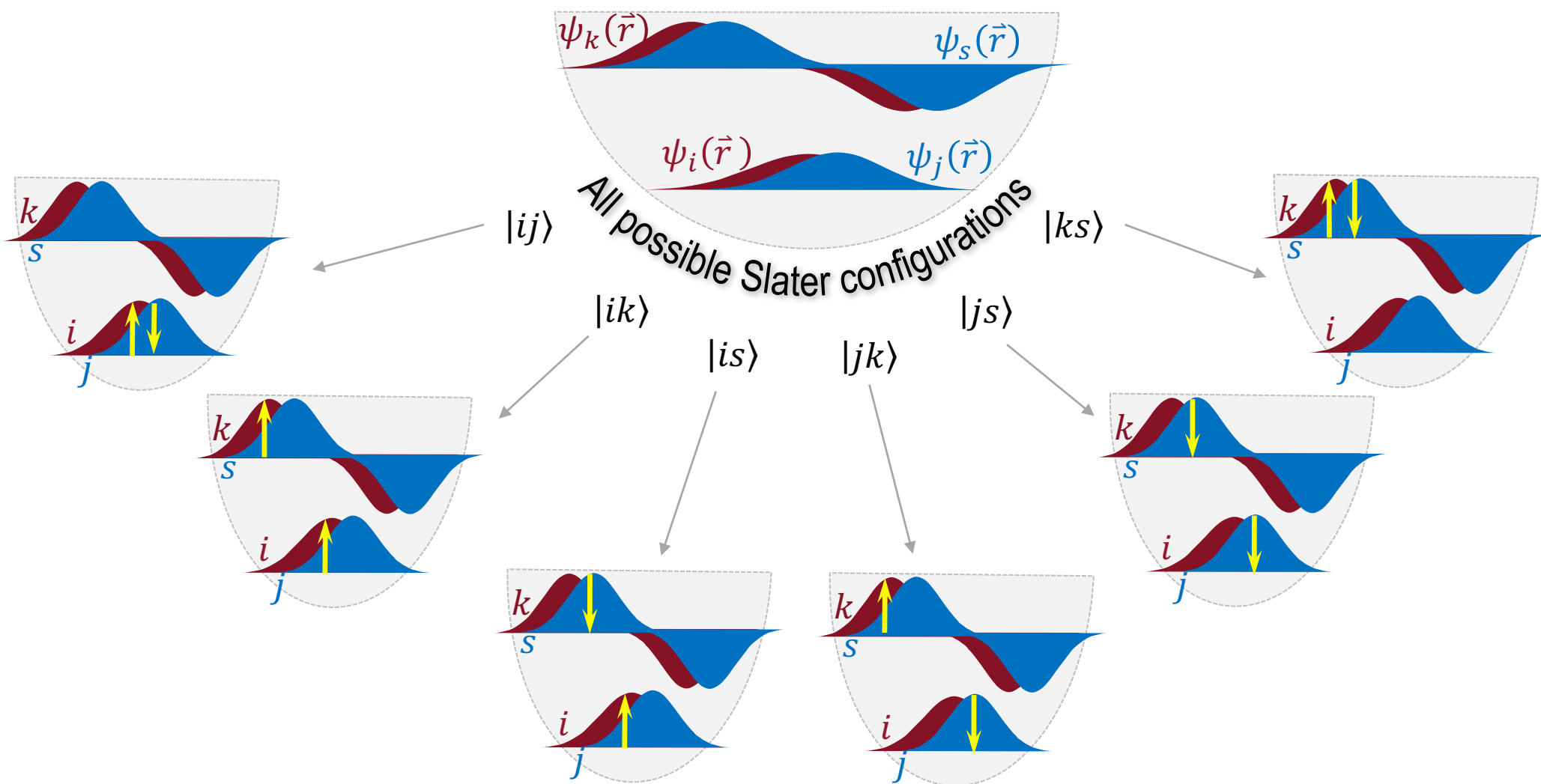
~~Indistinguishable electrons~~

$$\Psi_{ij}(\vec{r}_a, \vec{r}_b) = \begin{vmatrix} \psi_i(\vec{r}_a) & \psi_j(\vec{r}_a) \\ \psi_i(\vec{r}_b) & \psi_j(\vec{r}_b) \end{vmatrix} = |ij\rangle$$

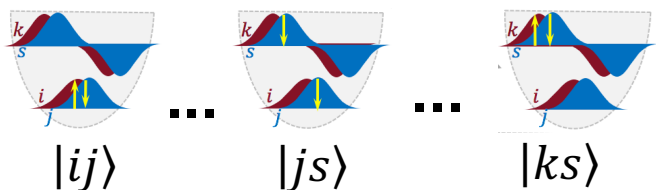
Slater Determinant

2 indistinguishable electrons
2 single-electron wavefunctions

Complete set of single-electron states



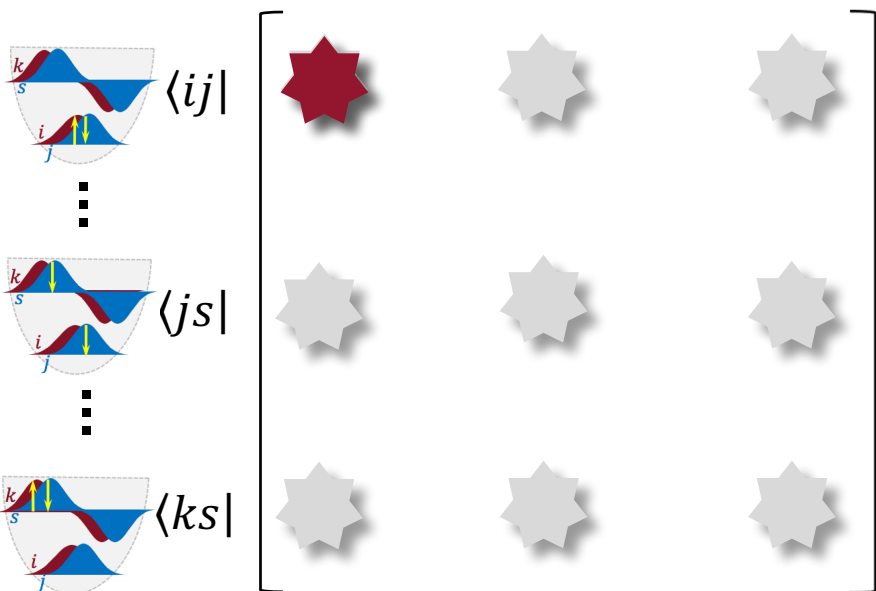
Complete set of Slater determinants as basis for two-electron Hamiltonian



$$\star \langle ij | \mathcal{H} | ij \rangle$$

$$\langle ij | \mathcal{H}^{(1)} | ij \rangle + \langle ij | \mathcal{H}^{(2)} | ij \rangle$$

$$E_i + E_j + \langle ij | \frac{1}{|\vec{r}_a - \vec{r}_b|} | ij \rangle$$



Single electron in ψ_i

Single electron in ψ_j

Interactions between electrons in ψ_i and ψ_j

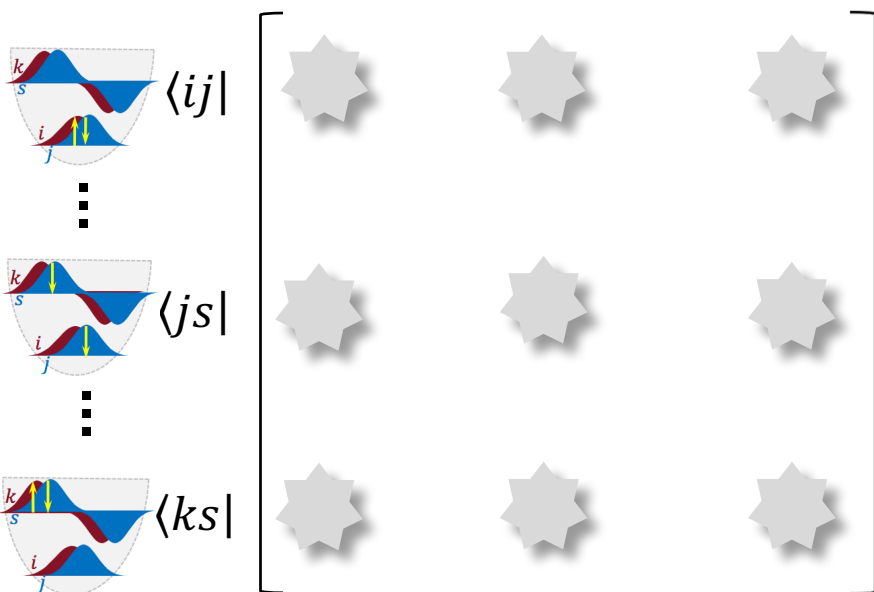
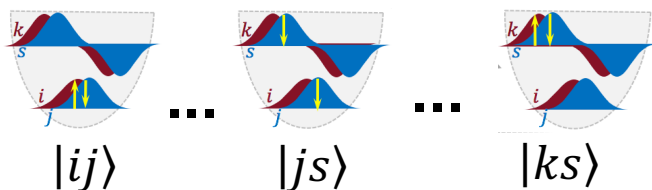
➤ Coulomb Interactions

$$\iint_V \psi_i^*(\vec{r}_a) \psi_j^*(\vec{r}_b) \frac{1}{|\vec{r}_a - \vec{r}_b|} \psi_i(\vec{r}_a) \psi_j(\vec{r}_b) d\vec{r}_a d\vec{r}_b$$

➤ Exchange Interactions

$$\iint_V \psi_i^*(\vec{r}_a) \psi_j^*(\vec{r}_b) \frac{1}{|\vec{r}_a - \vec{r}_b|} \psi_j(\vec{r}_a) \psi_i(\vec{r}_b) d\vec{r}_a d\vec{r}_b$$

FCI is EXACT in the space spanned by the basis

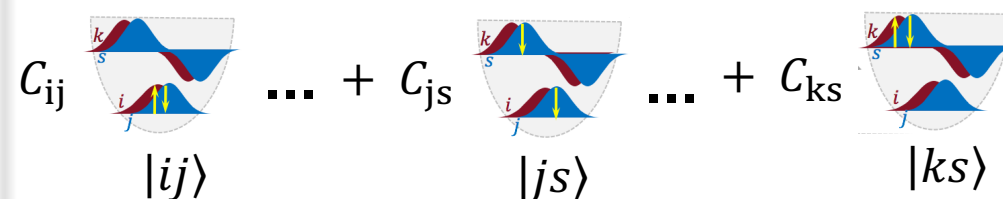


Eigensolvers: **LAPACK** + **FEAST**

✓ Faster than using either one

Two-electron energy levels

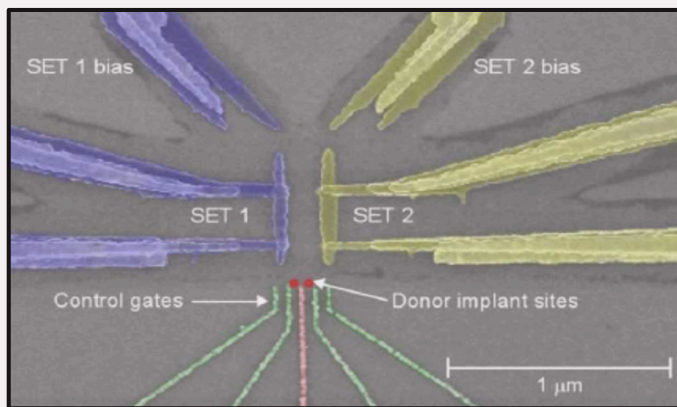
Two-electron wavefunctions



Exact **Spectrum** and **Configuration** of multi-electron states from FCI

Single-Electron States

Atomistic Tight-Binding



- ✓ Multi-million atom domain
- ✓ Complex geometries
- ✓ Atomistic effects of interfaces
- ✓ Incorporate bandstructure effects

Two-Electron Slater Determinants

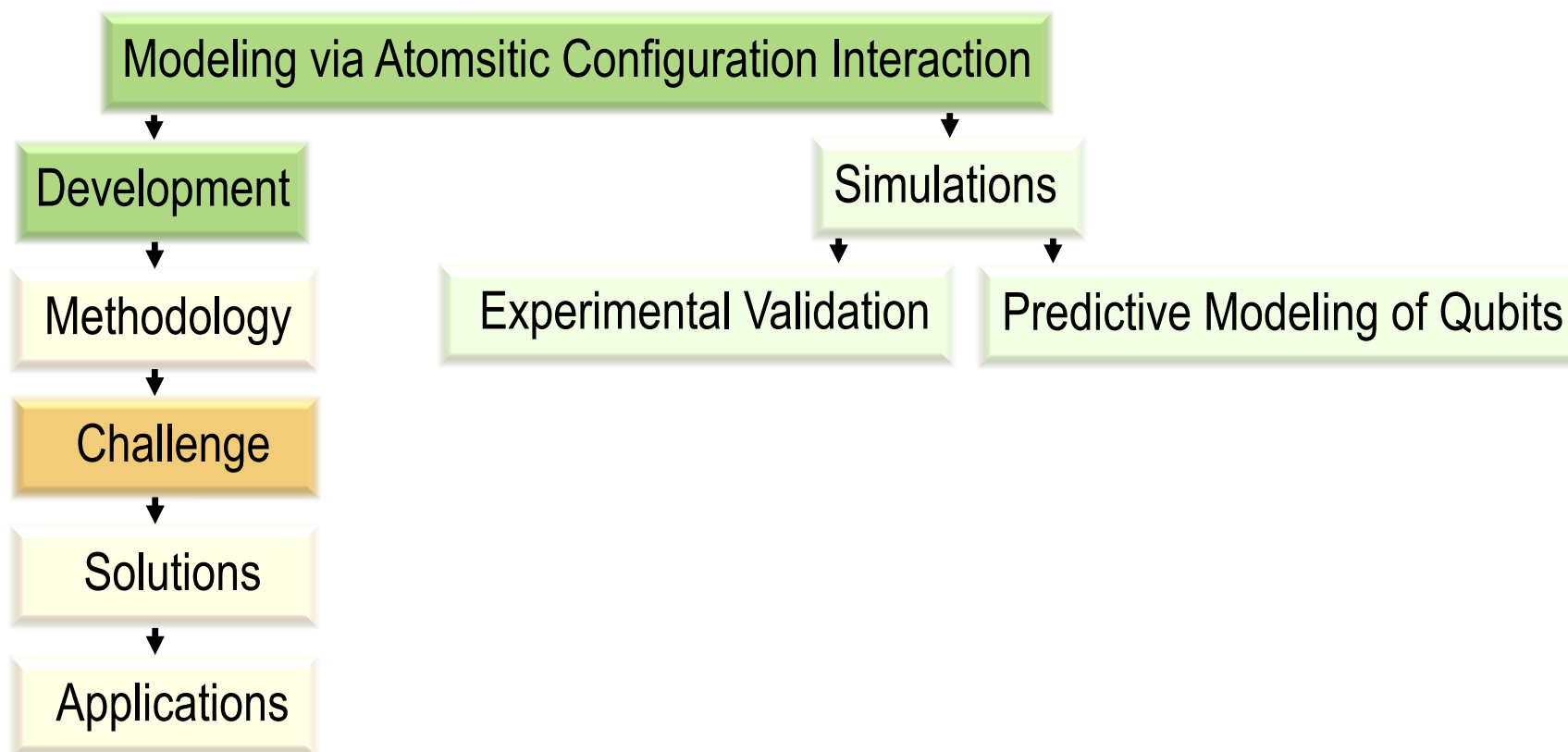
Full Configuration Interaction

- ✓ Coulomb repulsion
- ✓ Exchange interactions
- ✓ Correlations

Multi-Electron States

Atomistic Configuration Interaction (ACI) to model multi-electron devices

Electron Spin Qubits in Solid-State Architectures



Challenge: $\mathcal{O}(N^2 n^e)$

N : # atoms

n : # single-electron states in the basis
 e : # electrons

ACI matrix elements

$$\iint_V \psi_i^*(\vec{r}_a) \psi_j^*(\vec{r}_b) \frac{1}{|\vec{r}_a - \vec{r}_b|} \psi_k(\vec{r}_a) \psi_l(\vec{r}_b) d\vec{r}_a d\vec{r}_b$$

✗ Double integrals over all atoms in the simulation domain

$\mathcal{O}(N^2)$

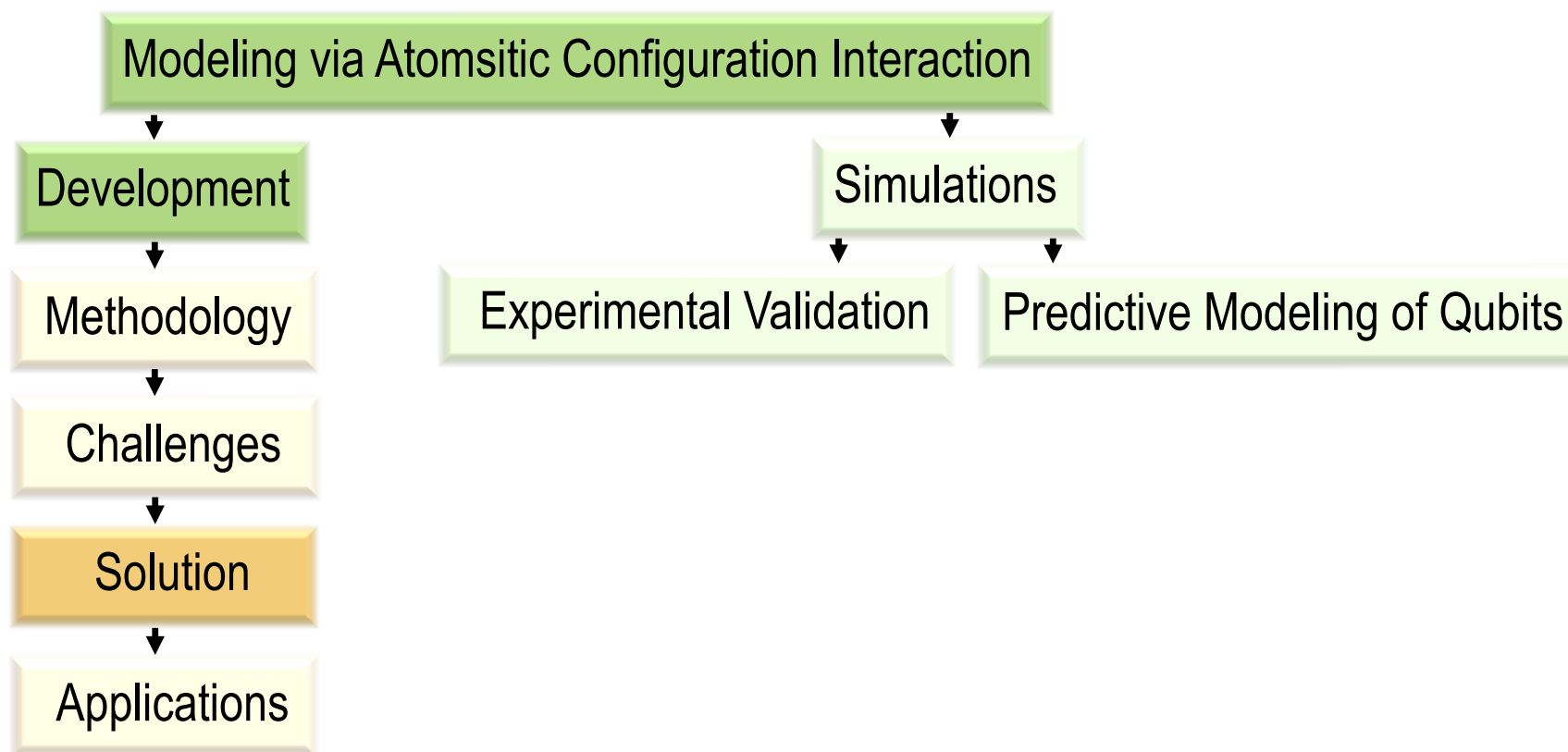
Slater determinants in ACI basis


e electrons n in states: ${}^n_e C$

$\mathcal{O}(n^e)$

ACI is computationally intensive for large N or n or e

Electron Spin Qubits in Solid-State Architectures



Challenge: $\mathcal{O}(N^2 n^e)$ 

Solution 1:

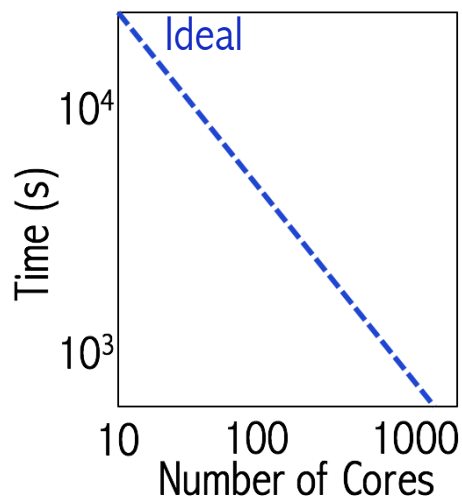
High Performance Computing
Parallelize data and computations

Solution 2:

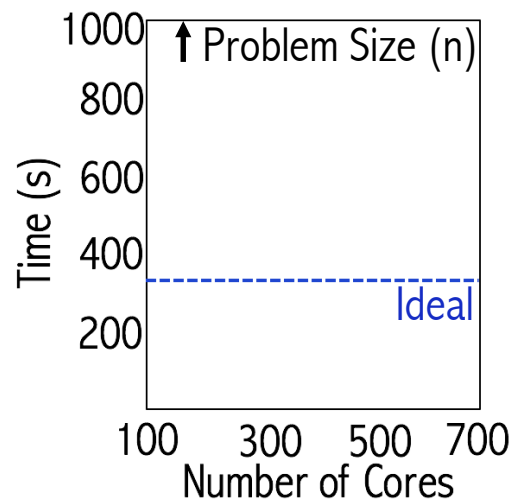
Optimized Algorithms
Complexity Reduction from N^2 to $N \log N$

“Efficiently” distribute the data and computations to several CPUs

Strong Scaling



Weak Scaling

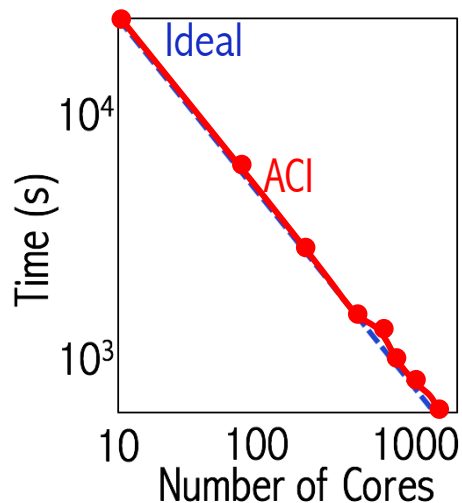


Overhead

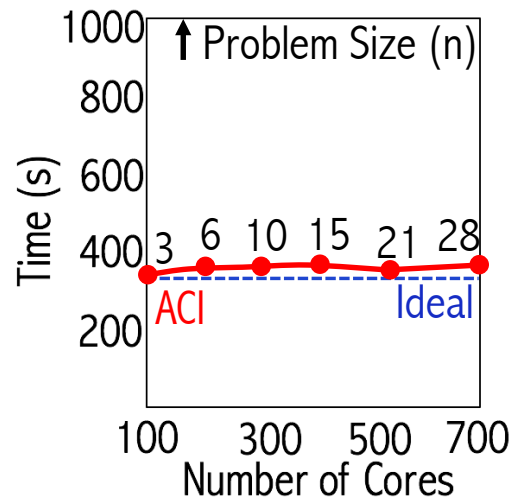
< 5%
IO and communication

“Efficiently” distribute the data and computations to several CPUs

Strong Scaling




Weak Scaling



Overhead

< 2%
IO and communication

ACI scales close to ideal

Challenge: $\mathcal{O}(N^2 n^e)$ 

Solution 1:

High Performance Computing

Parallelize data and computations

Solution 2:

Optimized Algorithms

Complexity Reduction from N^2 to $N \log N$

Identify the most demanding computations

$$\langle ij | kl \rangle = \iint_V \psi_i^*(\vec{r}_a) \psi_j^*(\vec{r}_b) \frac{1}{|\vec{r}_a - \vec{r}_b|} \psi_k(\vec{r}_a) \psi_l(\vec{r}_b) d\vec{r}_a d\vec{r}_b : 6D \text{ Integral !}$$

$$\sum_{a=1}^N \sum_{b=1}^N Q_{ik}(\vec{r}_a) \frac{1}{|\vec{r}_a - \vec{r}_b|} Q_{jl}(\vec{r}_b)$$

Mathematically similar in form to the very well known **N-Body Problem!**

Interactions between **EVERY** pair of particles of an N-particle system

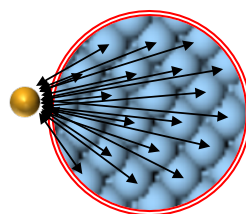
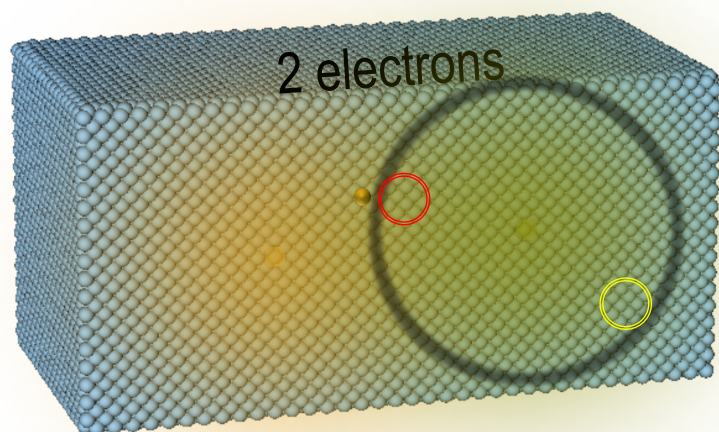
masses : Gravitation

atoms : Molecular Dynamics

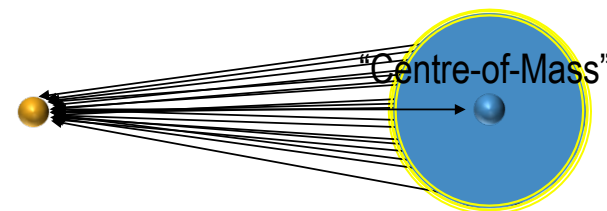
charges : Electrodynamics

Fast Multipole Method for N-Body problems

Acclaimed as one of the top 10 algorithms of the 20th century
 $O(N^2)$ complexity to $O(N \log N)$ or $O(N)$



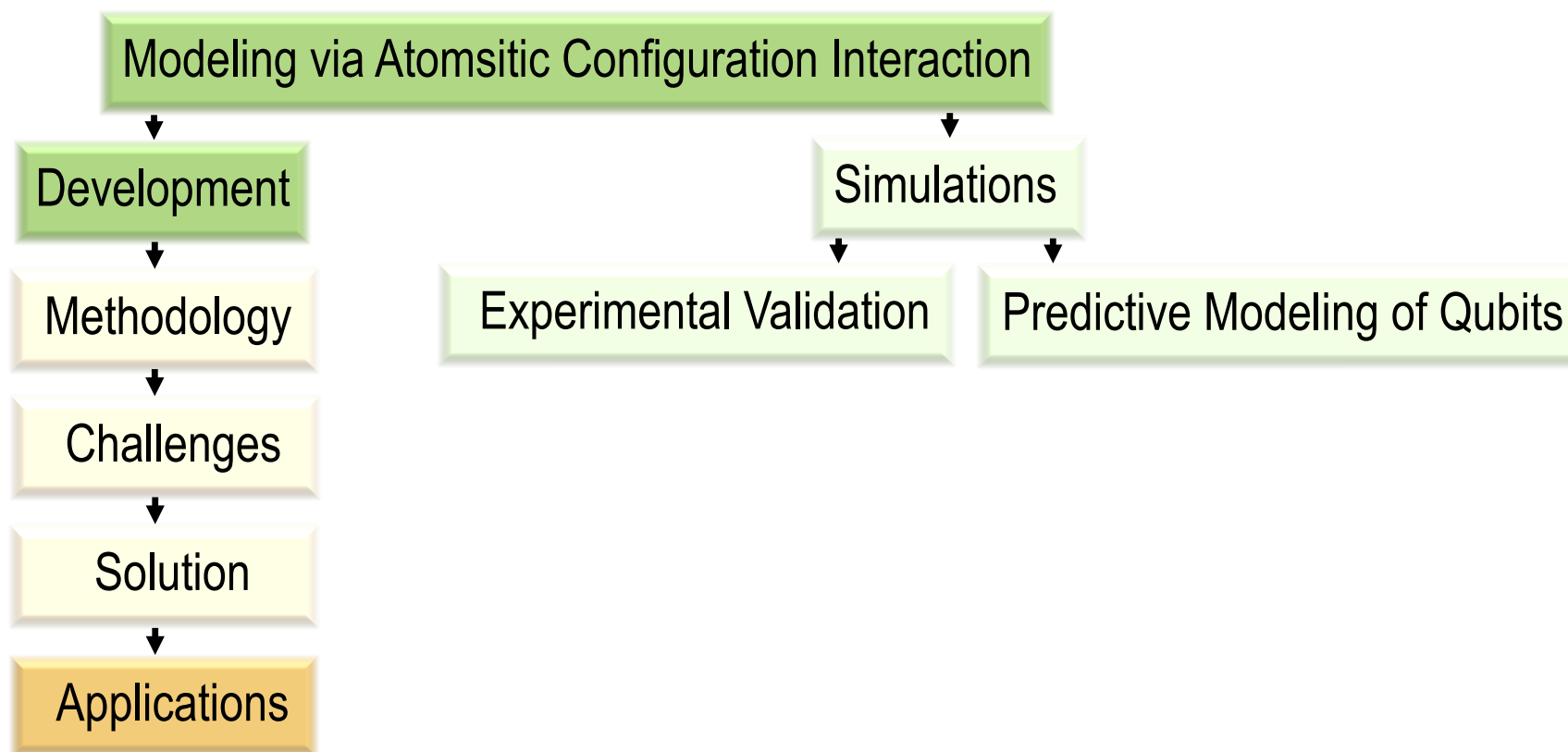
Particle-Particle
Interaction



Averaged effective interaction
from the far away atoms

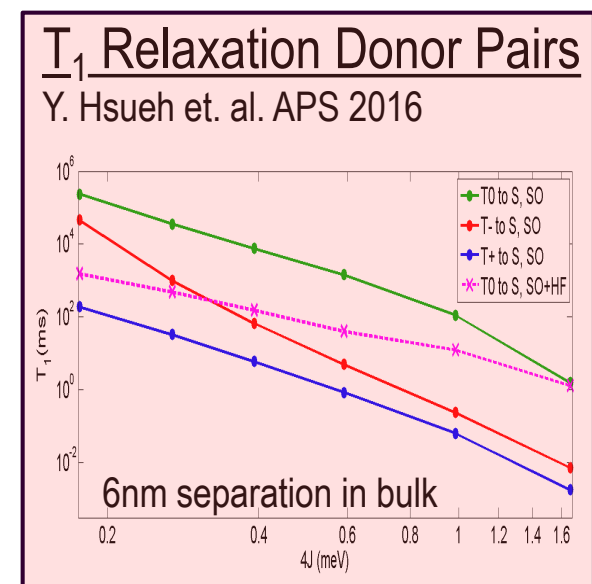
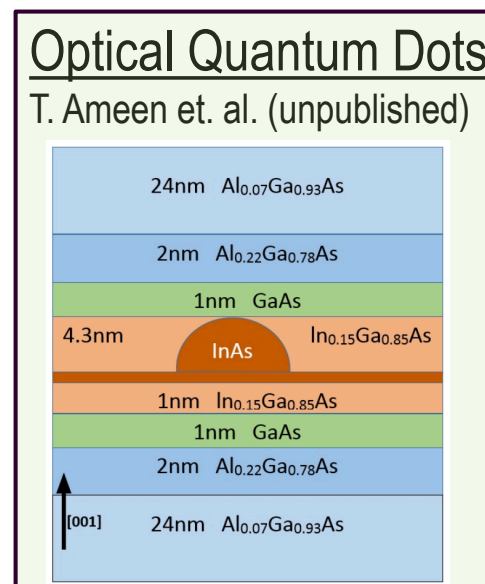
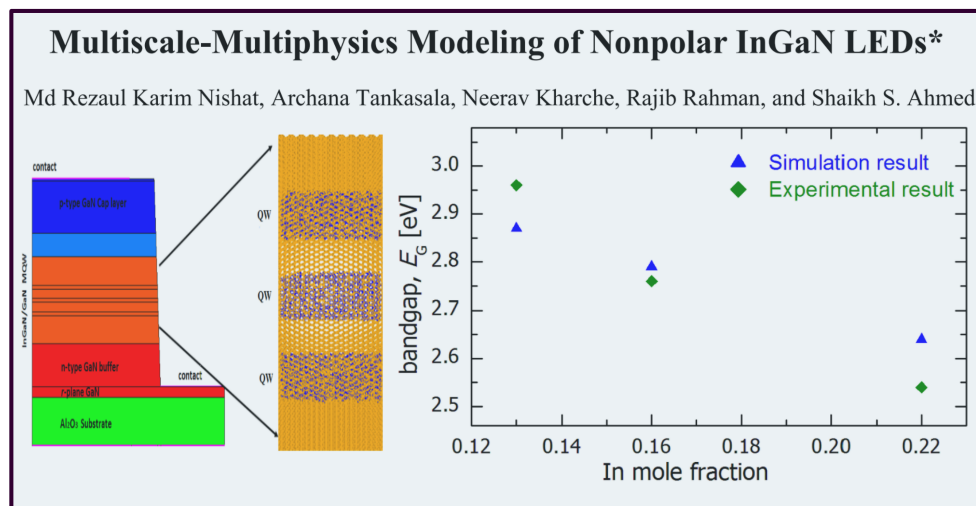
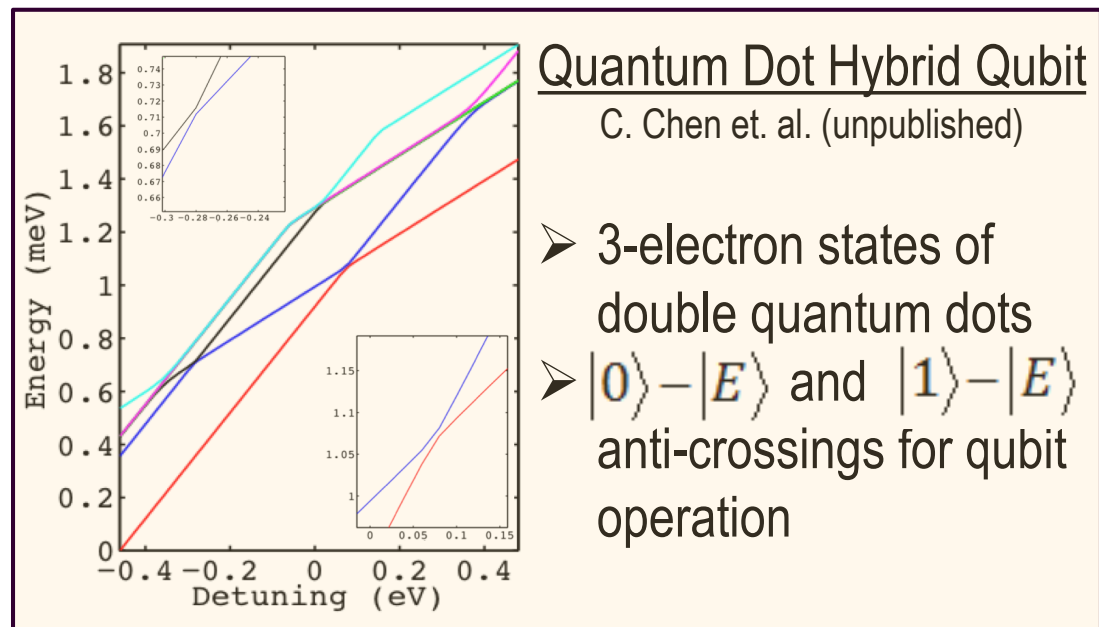
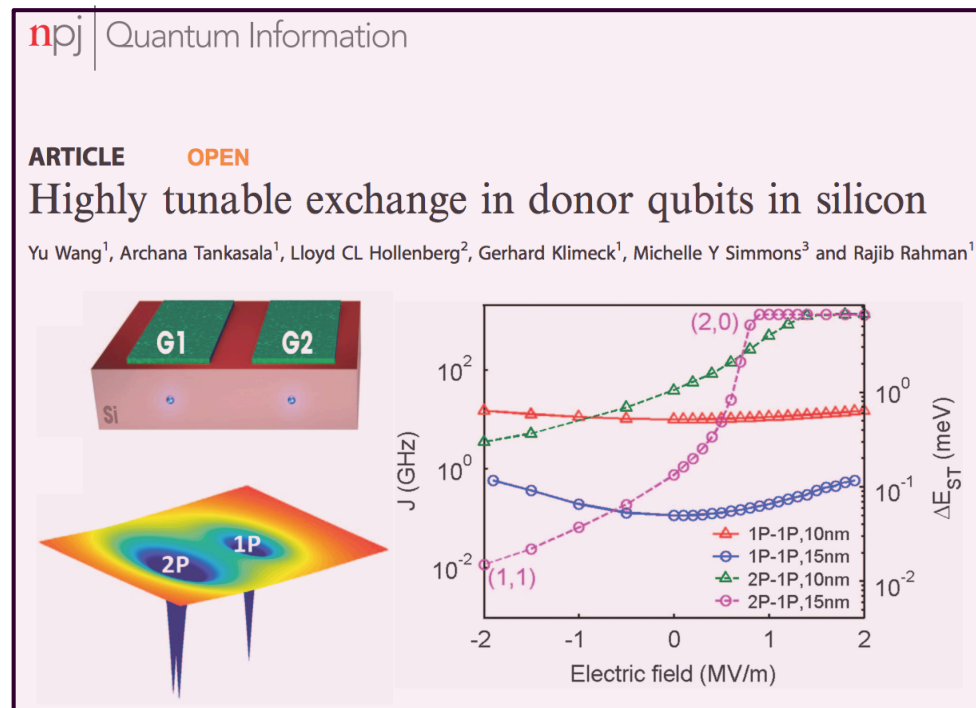
Upto 100x speed up in ACI achieved with Fast Multipole Method

Electron Spin Qubits in Solid-State Architectures

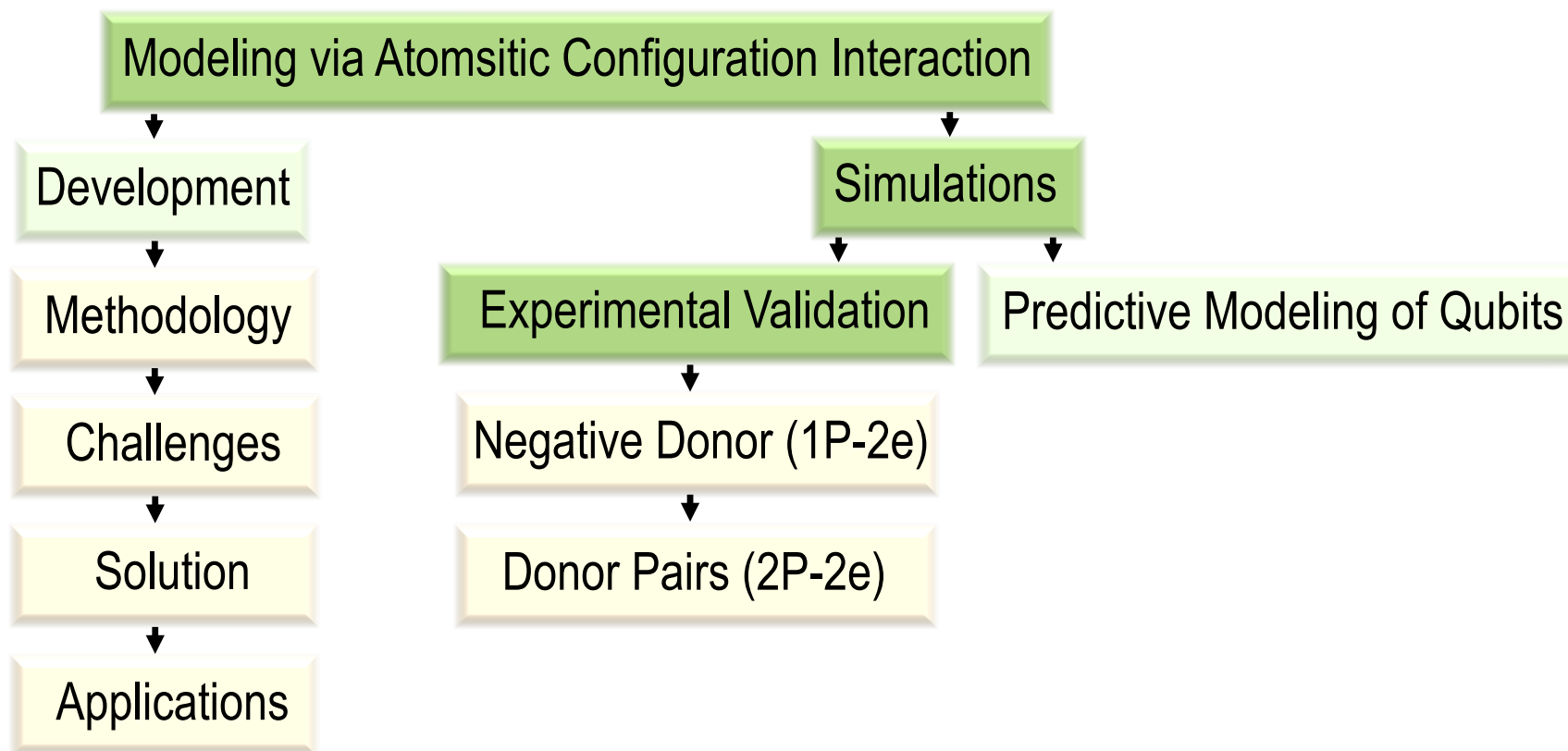


Accurately model electron-electron interaction in realistic quantum computing devices

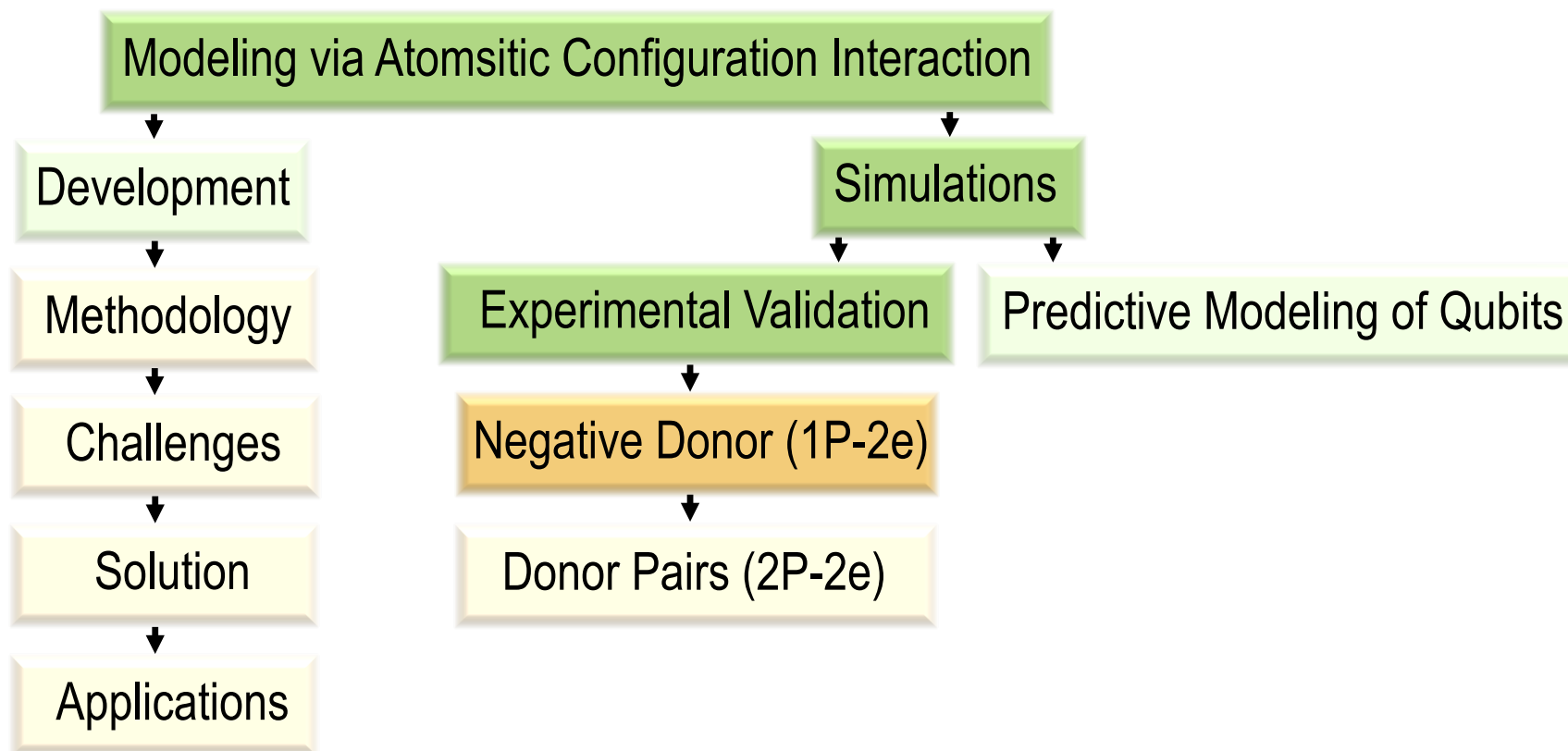


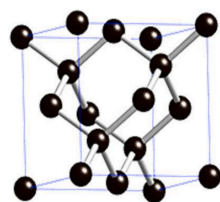
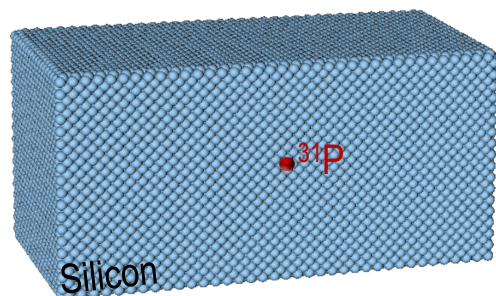


Electron Spin Qubits in Solid-State Architectures

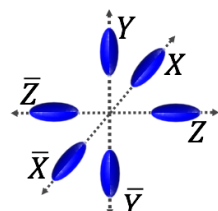


Electron Spin Qubits in Solid-State Architectures

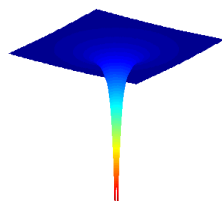




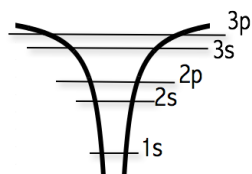
Tetrahedral Crystal Potential



Conduction Valleys

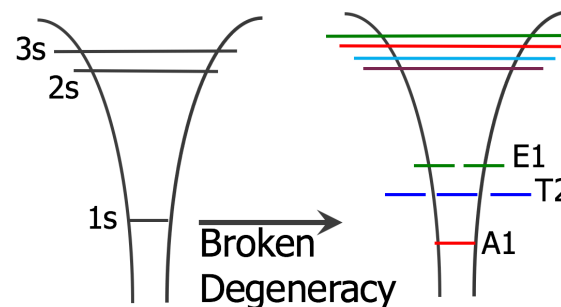


Donor Coulomb Potential



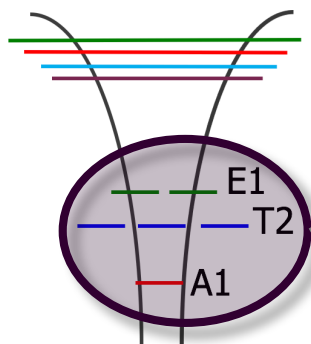
Hydrogenic Levels

Valley-Orbit Coupling



Atomistic Tight-Binding accurately captures the single electron energy spectrum of donor

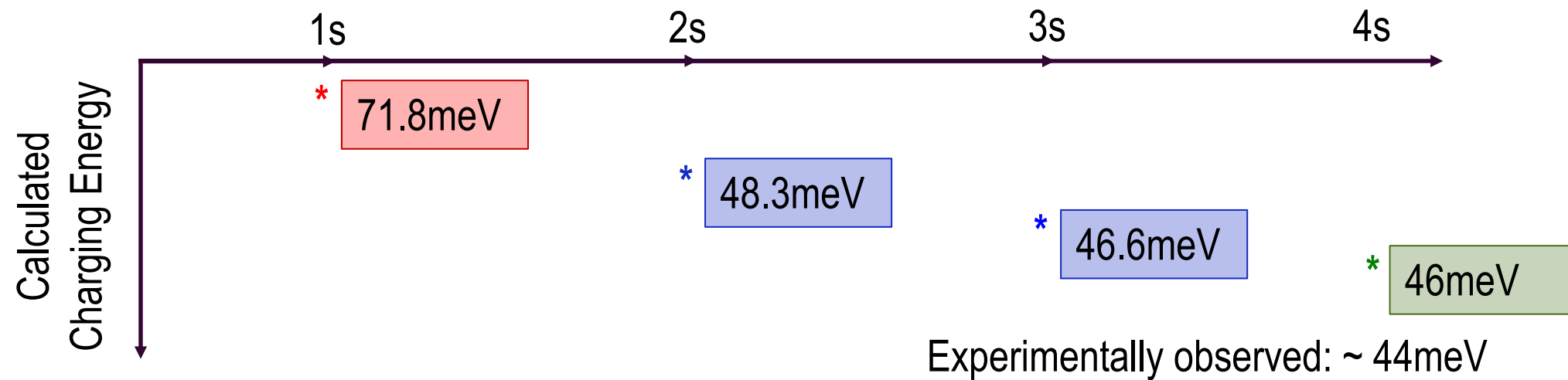
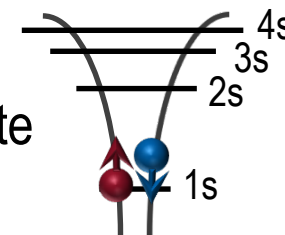
Energy spectrum of a donor in silicon



Typically considered for D^- calculation

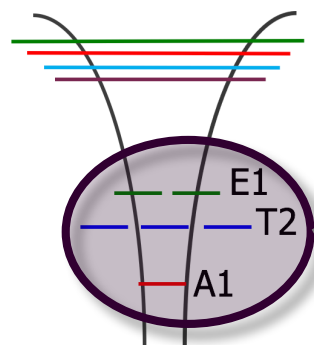
Assumption:

Both electrons in 1s-like state



Two-electron charging energy of single donor matches with experiments

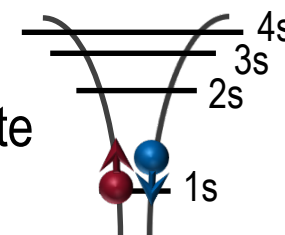
Energy spectrum of a donor in silicon



Typically considered for D^- calculation

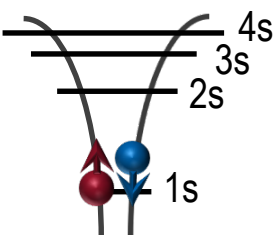
Assumption:

Both electrons in 1s-like state

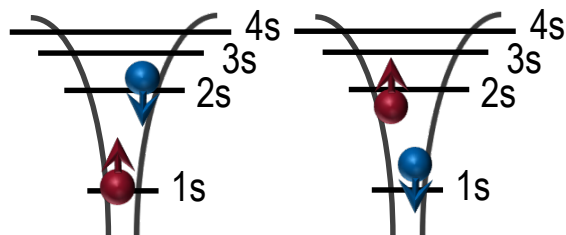


Two-electron wavefunction from ACI

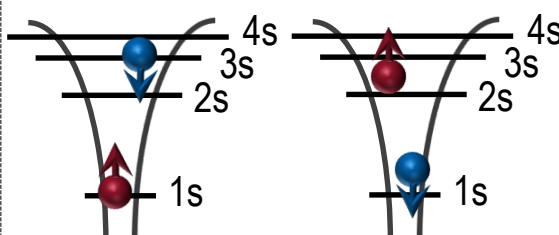
37%



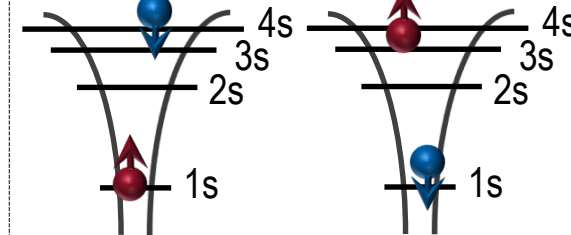
56%



6%

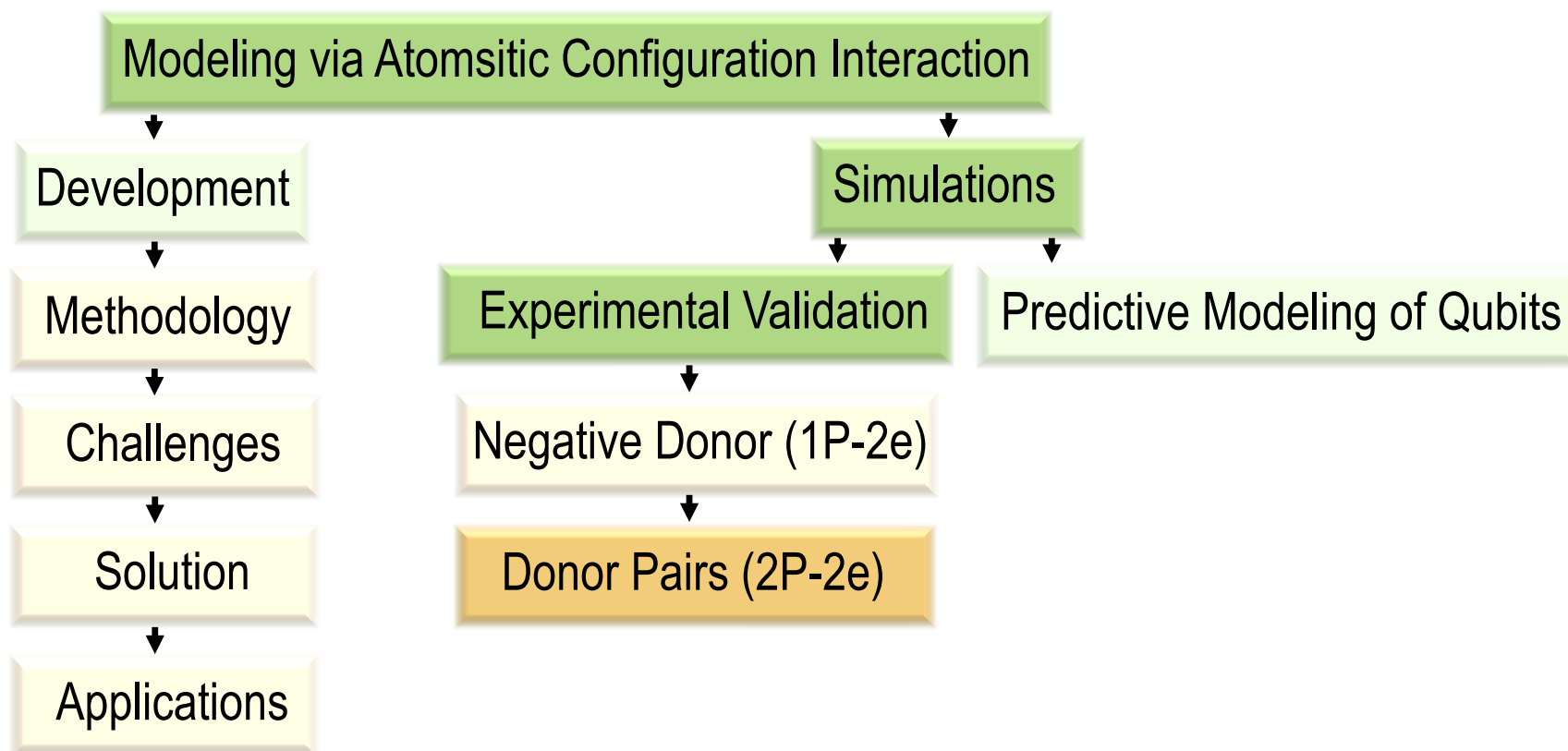


1%



ACI gives the configuration of the two-electron state of a bulk donor

Electron Spin Qubits in Solid-State Architectures



Example: **SWAP Operation**



Electron-electron interactions in donor pairs: Two qubit operations

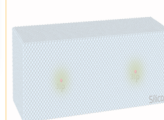
Electron spins rotate in presence of each other

When to stop applying the gate bias?

➤ Speed of electron spin rotation → [Electron-Electron Interaction](#)

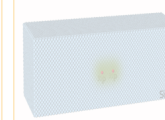
✓ Two Qubit operations rely on interaction strength between two electrons

[Electron-Electron Interactions](#) must be accurately estimated for precise qubit control



Heitler-London Approximation

✓ Well separated donors



Hartree-Fock Approximation

✓ Closely spaced donors

Realistic Quantum Computing Devices

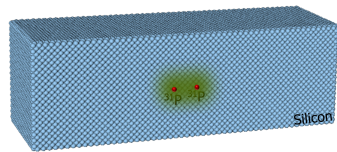
Donor separations range from [1nm \(donor clusters\)](#) to [25nm \(spin qubit\)](#)

Available models **NOT valid** over all donor separation regimes and are only **approximate**

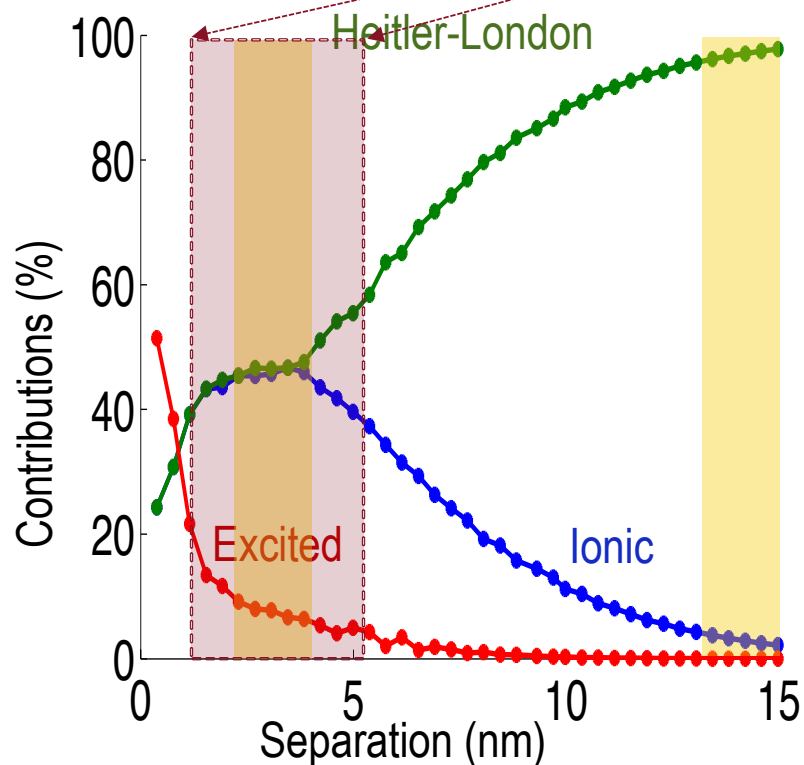
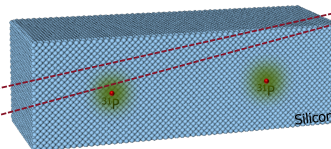
Exact electron-electron interactions for precise qubit control

[Model to capture electron-electron interactions accurately for ALL donor separations](#)

Hartree-Fock Regime



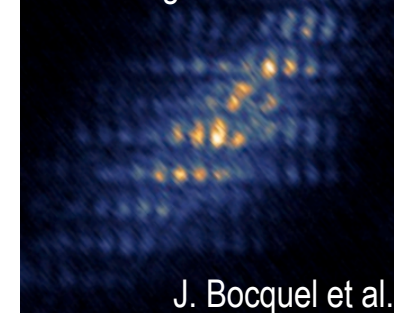
Heitler-London Regime



STM Experiments on donor pairs

CENTRE FOR
QUANTUM COMPUTATION &
COMMUNICATION TECHNOLOGY
AUSTRALIAN RESEARCH COUNCIL CENTRE OF EXCELLENCE

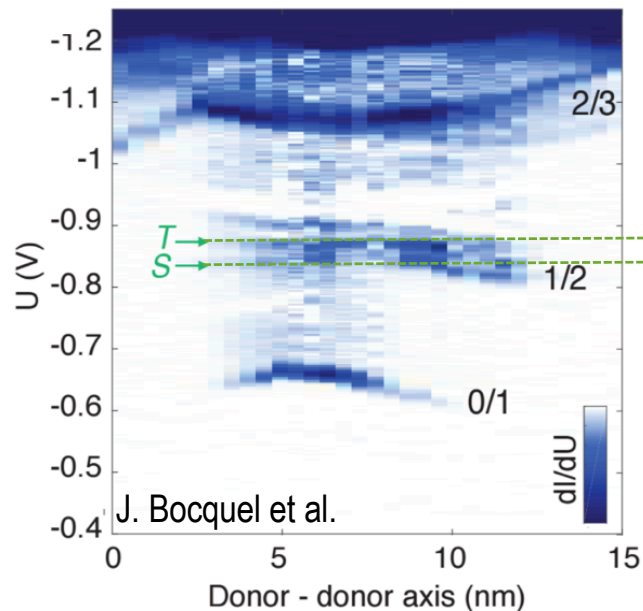
STM Image of Donor Pair



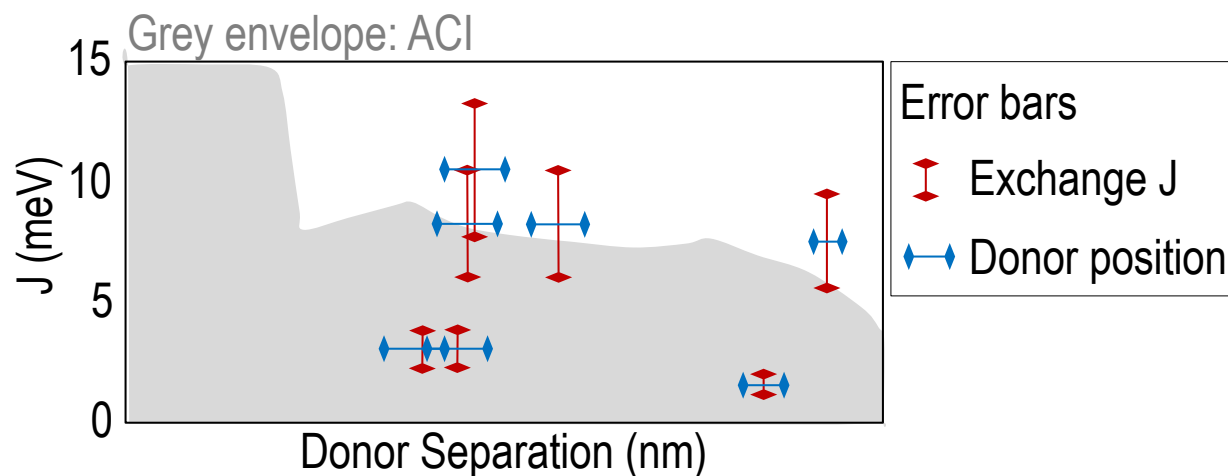
J. Bocquel et al.

Closely spaced donors 2nm-5nm

Approximate models invalid for donors in STM experiments

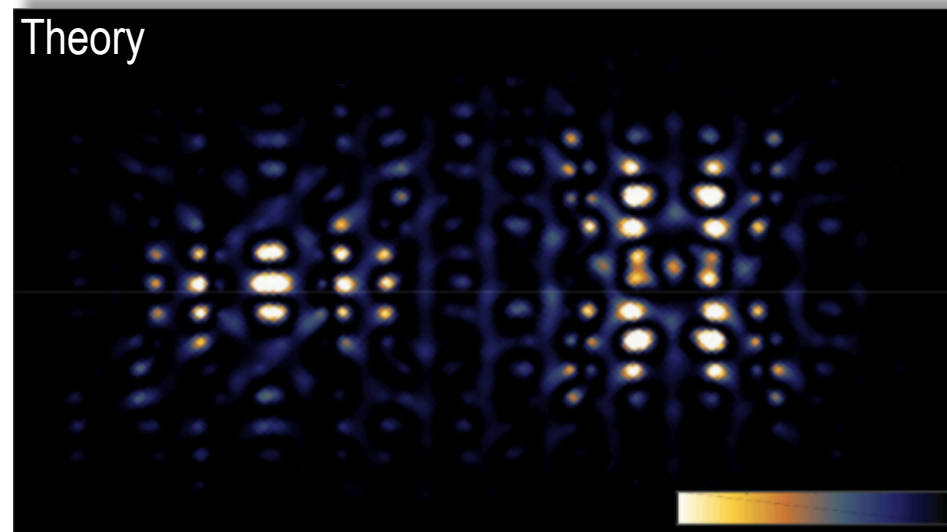
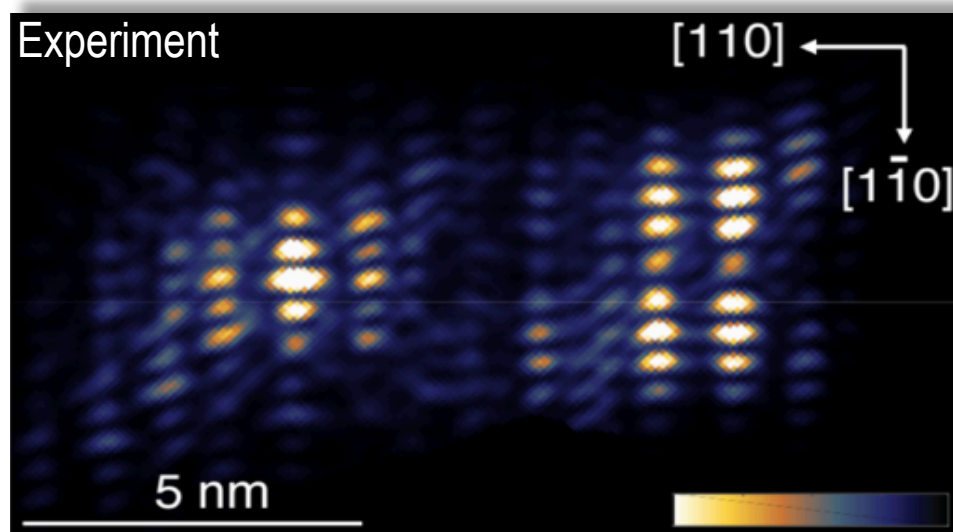


Exchange for several donor pairs:



Exchange from ACI agrees well with the STM measurements

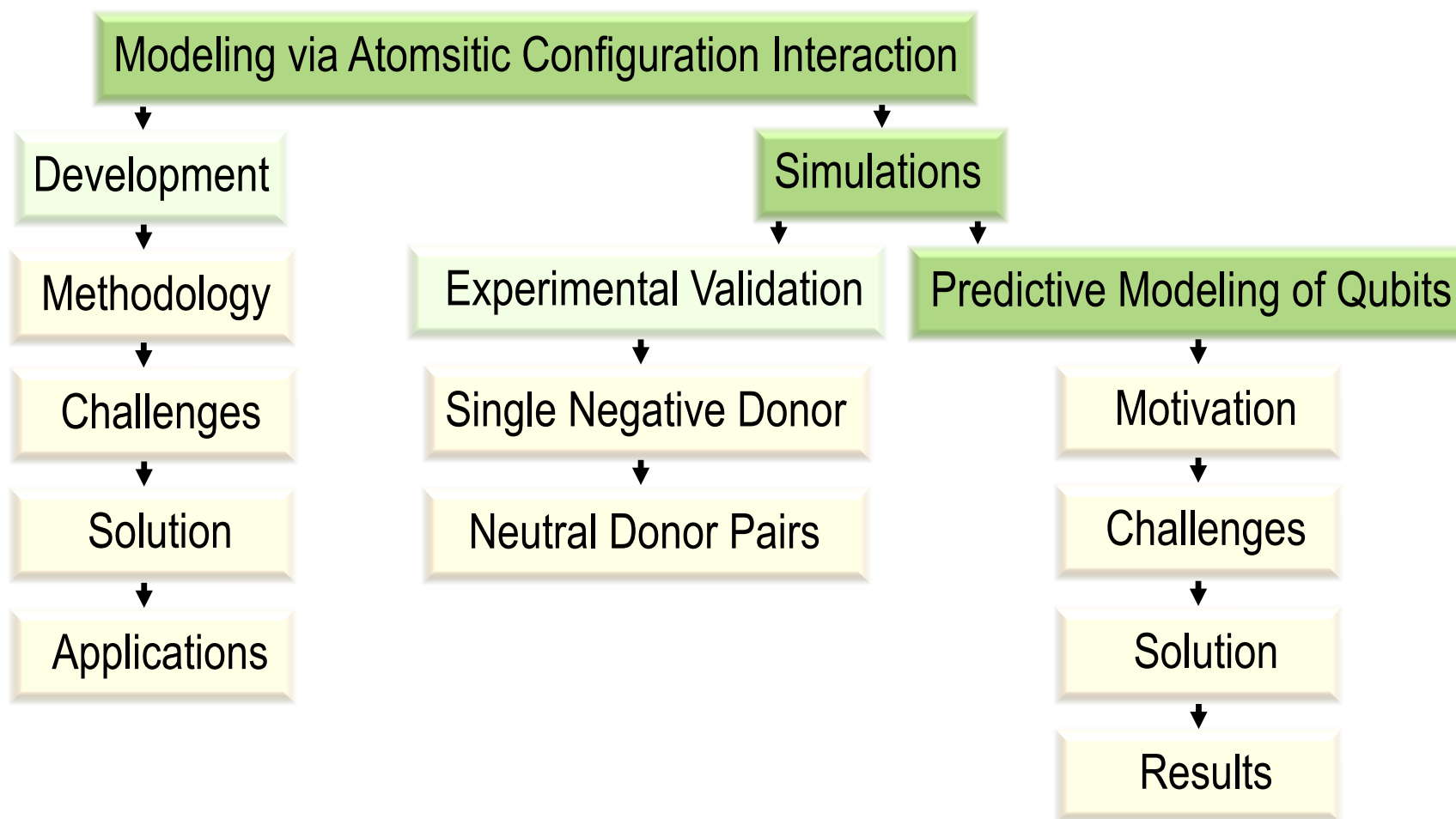
STM Image of donor pair corresponding to $2e \rightarrow 1e$ transition



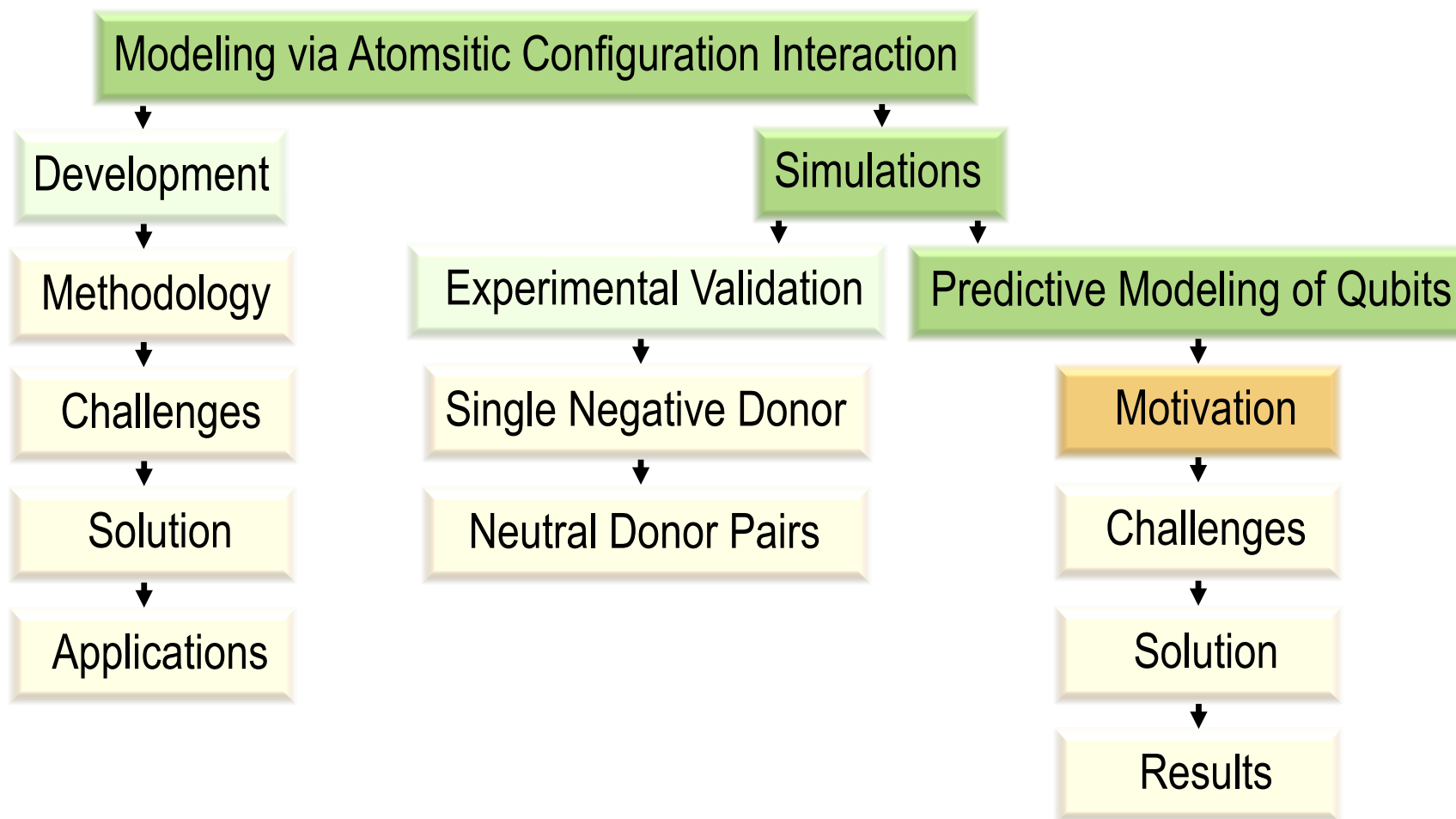
* Calculated by M. Usman from ACI wavefunctions

Real space $2e \rightarrow 1e$ images from ACI agree well with the STM images

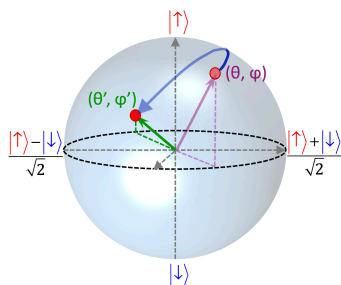
Electron Spin Qubits in Solid-State Architectures



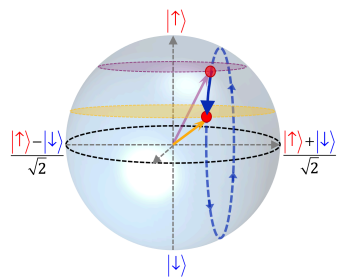
Electron Spin Qubits in Solid-State Architectures



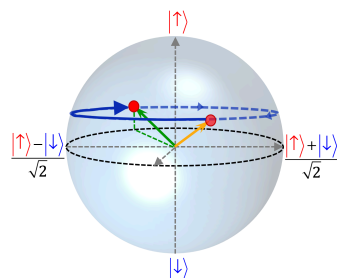
Arbitrary Rotation



Rotations about two fixed axes

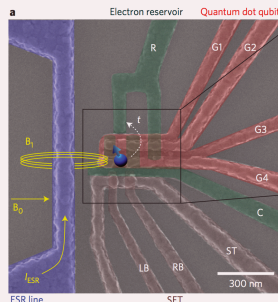


X-Rotation



Z-Rotation

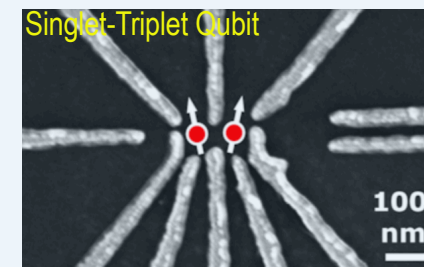
Single Spin Qubit



👎 Microwave Pulse

0.3 MHz

Two Spin Qubit

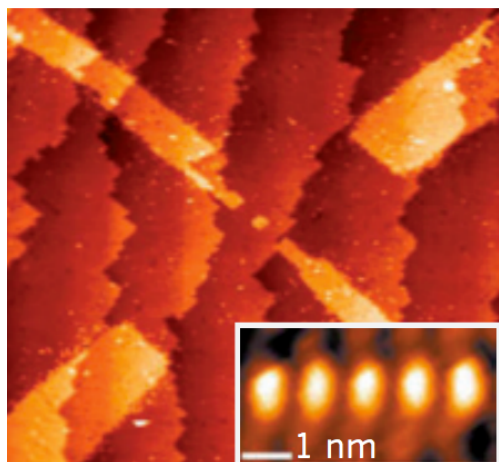
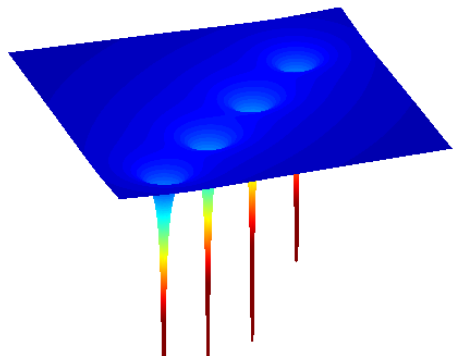


👍 Electrical Pulse

14 MHz
Isolated electrons

20 GHz
Interacting electrons

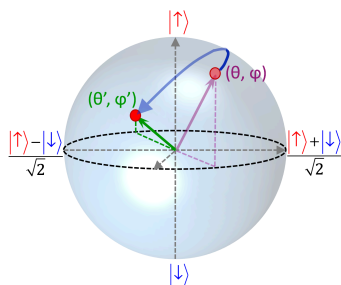
Two-spin qubits are faster due to electrical manipulation of **electron exchange interactions**



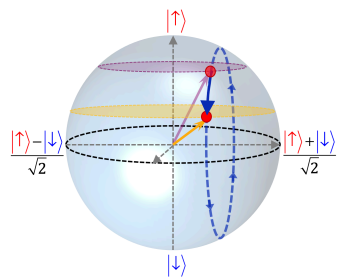
- Compatibility with current C-MOS technology
- Natural confinement of dopant atoms
- Consistency of dopant atom potentials in an atomically precise array as against lithographically defined dots
- STM lithography allows deterministic donor placement
- Extremely long spin coherence times
 - Electrostatic dots : $T_1 > 2\text{s}$ & $T_2 > 48\text{ms}$
 - Donors : $T_1 > 1000\text{s}$ & $T_2 > 0.5\text{s}$ at 1.8K

Donor bound electron spin qubits are promising towards scalable architectures

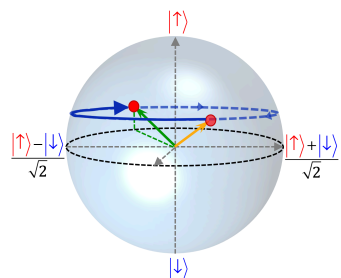
Arbitrary Rotation



Rotations about two fixed axes

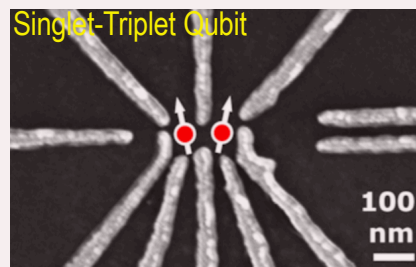


X-Rotation



Z-Rotation

Electrostatic Dots

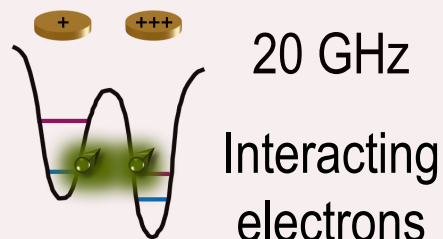


👍 Electrical Pulse



14 MHz

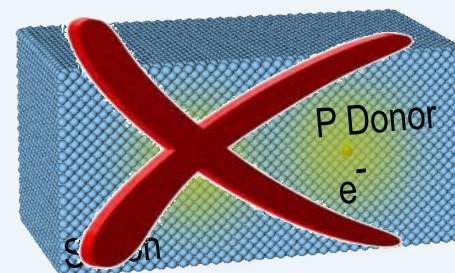
Isolated electrons



20 GHz

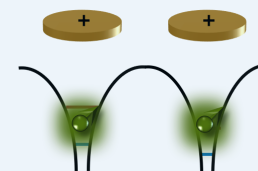
Interacting electrons

Donors in silicon

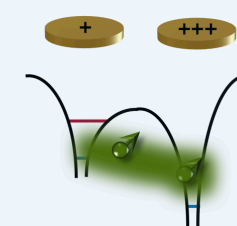


Feasible ?

👍 Electrical Pulse



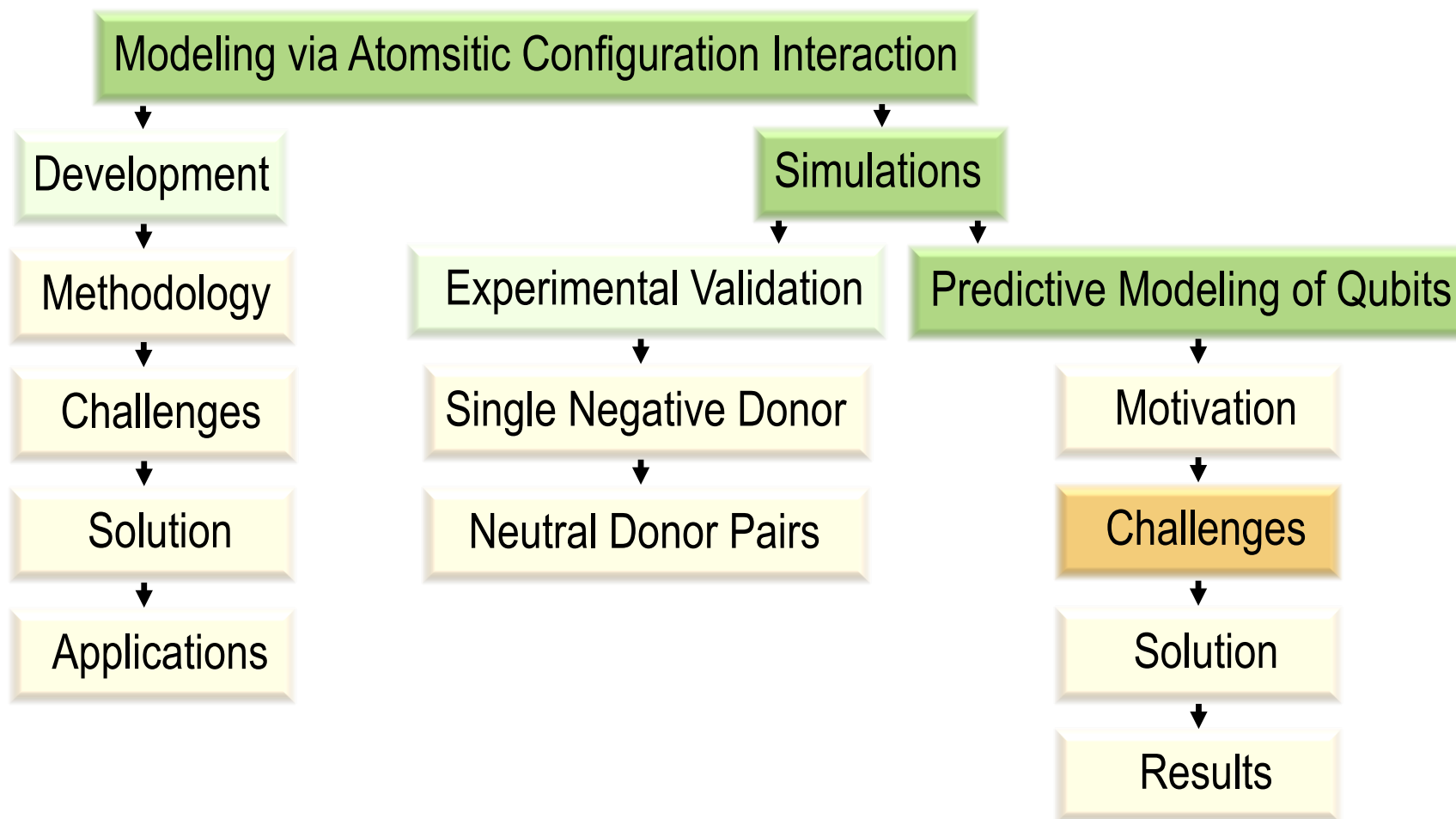
Fast ?



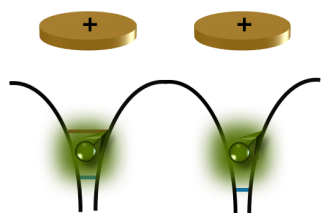
Fast ?

What are the challenges in realization of two-spin donor qubits?

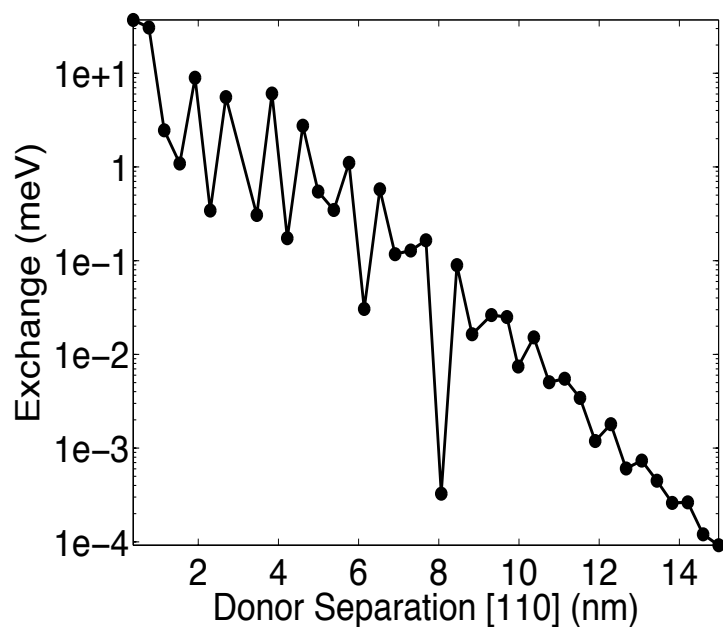
Electron Spin Qubits in Solid-State Architectures



Challenge 1: Exchange oscillations affect qubit manipulation



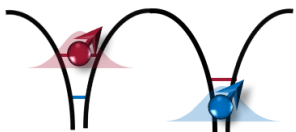
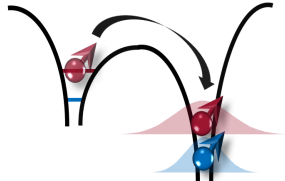

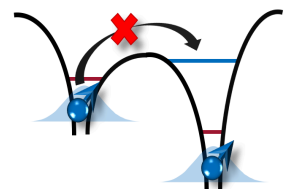
Electron exchange interactions control qubit operations



- Exchange interactions sensitive to donor positions
- Violent oscillations in electron exchange interactions

Demand precise gate control of electron interactions for a qubit operation

Challenge 2: Lack of bound triplets for qubit read-out

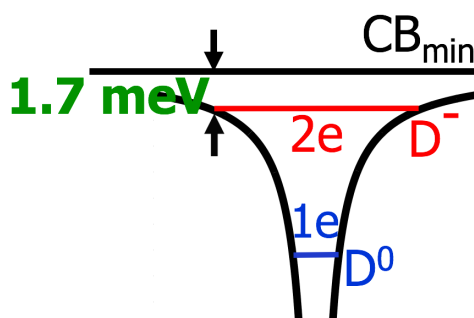
	Qubit State	Spin-to-Charge Conversion	# electrons
Singlet:			$(0_{\text{Left}}, 2_{\text{Right}})$
Triplet:			$(1_{\text{Left}}, 1_{\text{Right}})$

Charge sensing the dot for measurement

Bound Triplet States on **single donor** are important for qubit state read-out

Challenge 2: Lack of bound triplets for qubit read-out

Spectrum of Single Phosphorous Donor in Silicon



D^0 : Donor binding single electron

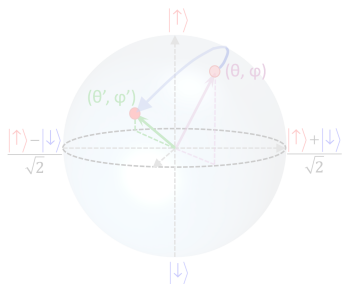
D^- : Donor binding two electrons

- 2-electron ground state is only **1.7 meV** from silicon CB_{\min}
- 2-electron excited states (triplets) are not bound

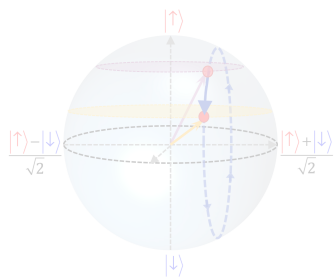
Difficult to confine two electrons on a donor in bulk silicon: No bound triplets

Challenge 3: Gradient magnetic fields for X-rotation of qubit

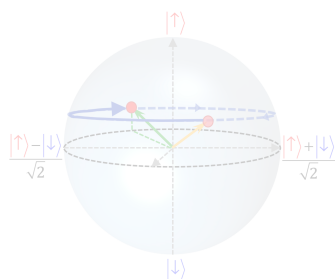
Arbitrary Rotation



Rotations about two fixed axes

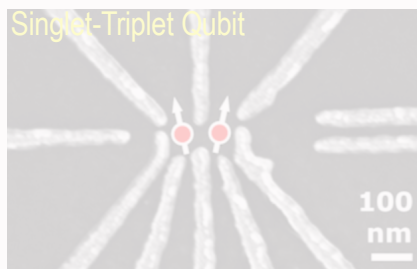


X-Rotation

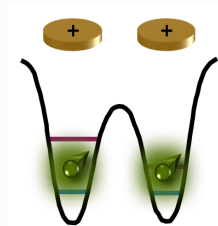


Z-Rotation

Two Spin Qubit

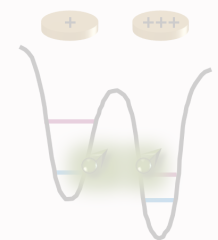


👍 Electrical Pulse



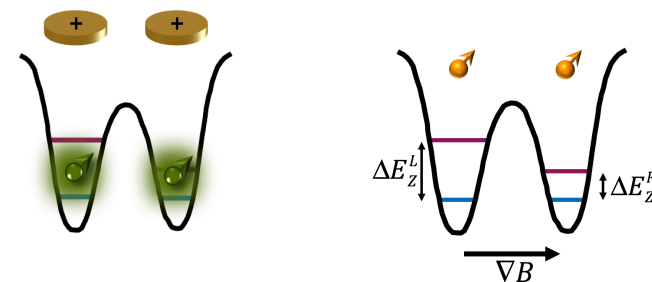
14 MHz

**Isolated
electrons**



20 GHz

**Interacting
electrons**

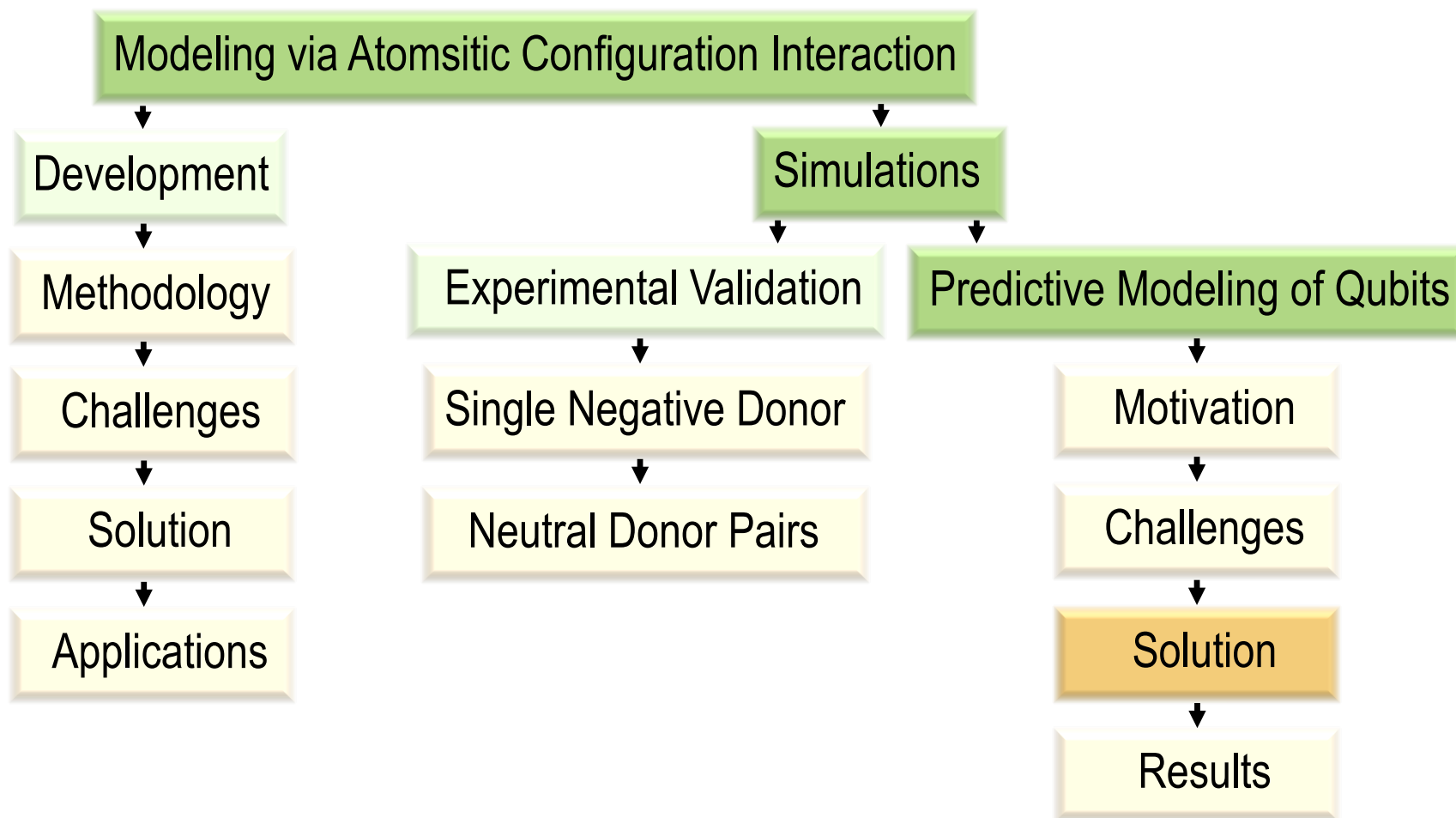


- Different Zeemann splitting in dots
- Isolated electrons evolve differently
- Develop a phase difference

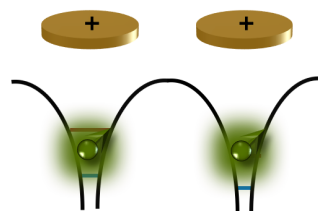
Gradient Magnetic Field

- ✗ Micromagnets
- ✗ Nuclear spins

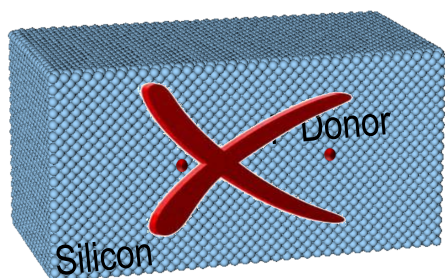
Electron Spin Qubits in Solid-State Architectures



Two Spin Qubit

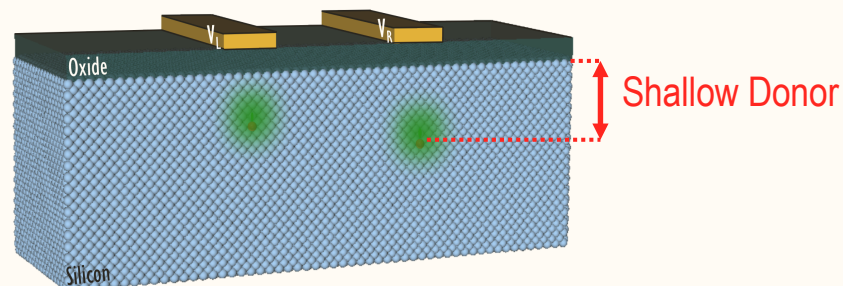


Donors in bulk silicon



SOLUTION

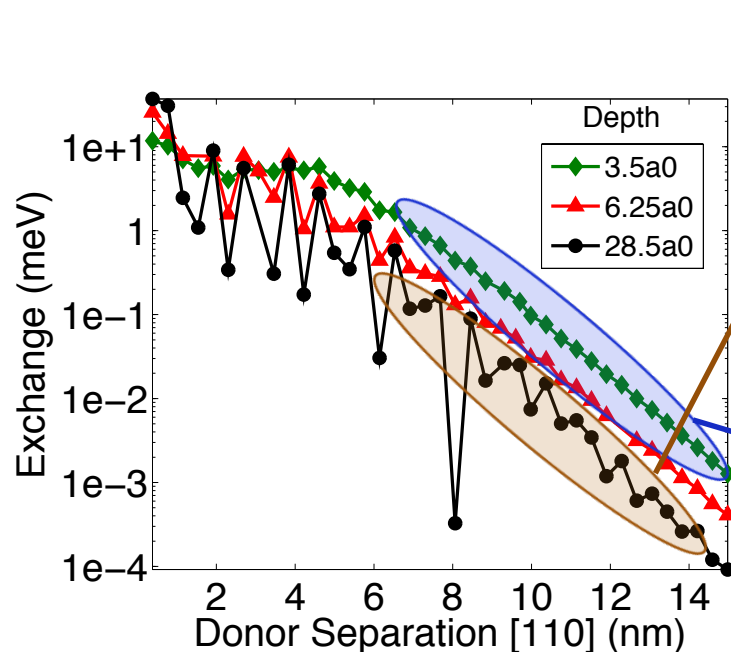
Sub-surface donors in silicon



Confine electrons to **SHALLOW dopant atoms** in silicon for two-spin qubits

Challenge 1: Exchange oscillations affect qubit manipulation

Solution : Exchange oscillations suppressed for shallow donors



Donors away from interface:

- X & Y valley interferences change with XY separation
- Causes oscillations in electron wavefunction overlap
- Oscillations in exchange interactions

Donors close to interface:

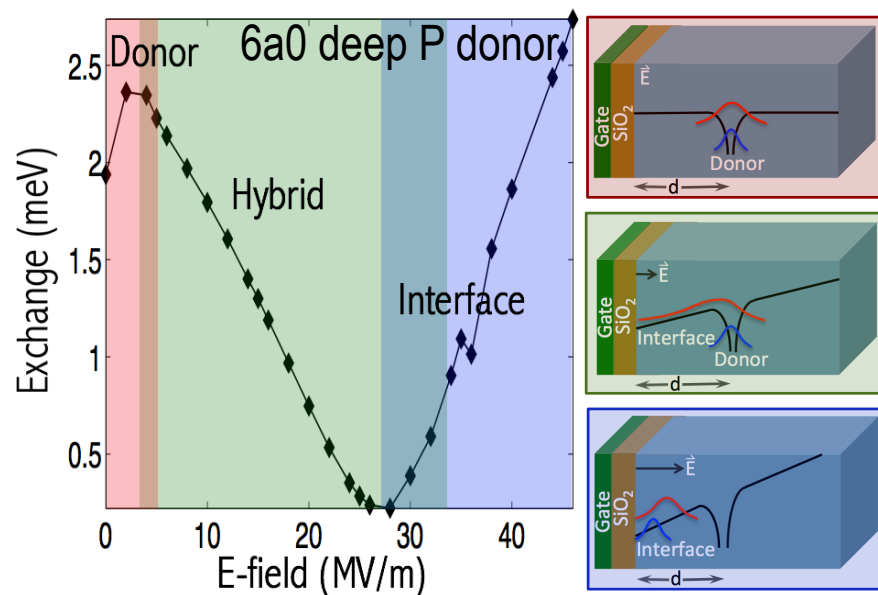
- Donor states Z valley dominant
- XY separation does NOT effect electron overlap
- Suppressed oscillations in exchange

Better gate control of electron exchange interactions due to suppressed oscillations

Challenge 2: Lack of bound triplets for qubit read-out

Solution : Bound triplets for shallow donors under applied fields

Singlet-Triplet splitting for sub-surface donor under applied gate field from ACI



Hybridized Regime (Moderate Fields):

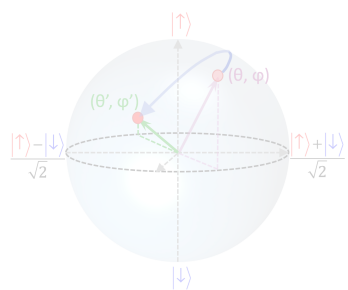
- ✓ Electrons can physically avoid one another
- ✓ Decreases electron exchange interactions: singlet-triplet splitting
- ✓ Triplets lower in energy and confined

Bound triplet states of shallow donors under electric fields allow multi-spin qubit read-out

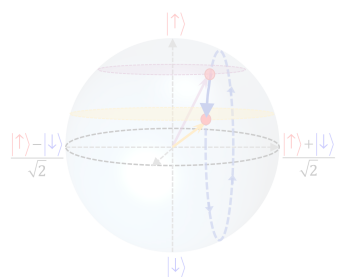
Challenge 3: Gradient magnetic fields for X-rotation of qubit

Solution : Tuning donor depth and fields for X-rotation

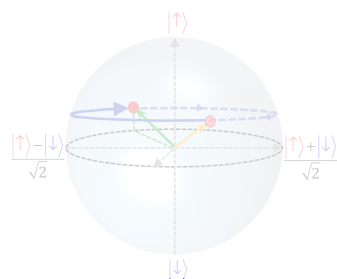
Arbitrary Rotation



Rotations about two fixed axes



X-Rotation

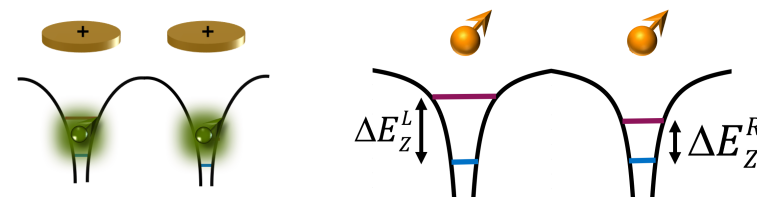
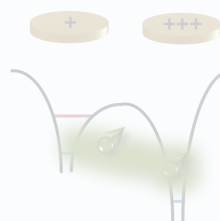
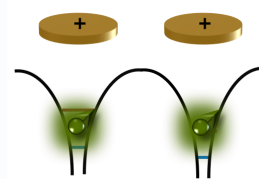


Z-Rotation

Donors in silicon



👍 Electrical Pulse

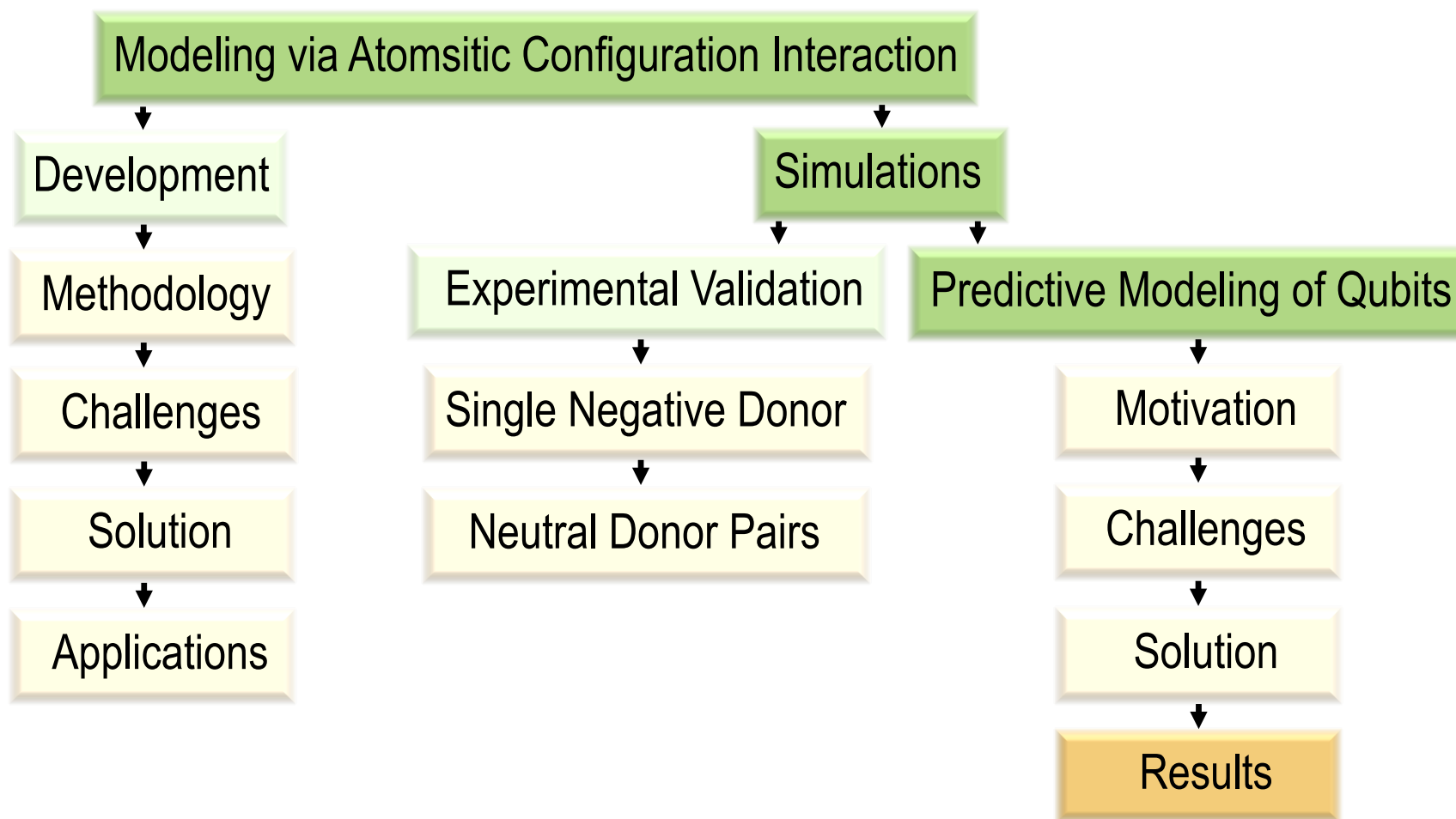


- Different Zeemann splitting in donors
- Isolated electrons evolve differently
- Develop a phase difference

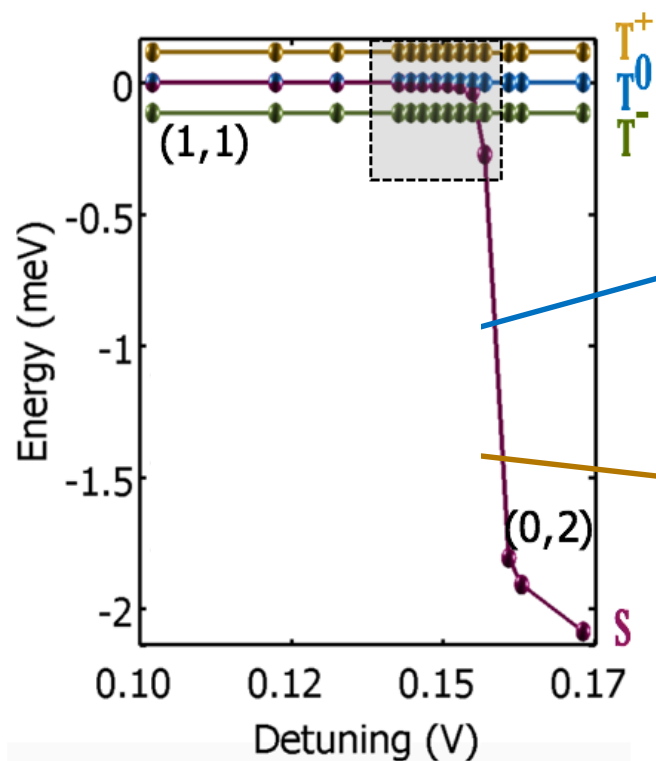
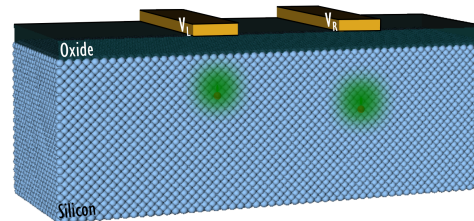
Electron g-factor difference

- ✓ Tuning donor depth
- ✓ Tuning gate biases

Electron Spin Qubits in Solid-State Architectures



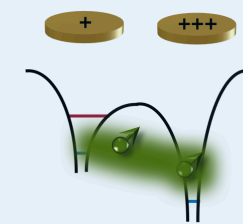
Two electron spectra from ACI



Qubit Manipulation

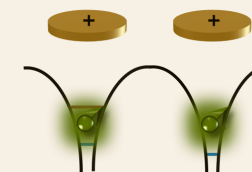
Large electron exchange

- ✓ Z Rotation
- ✓ 2 GHz



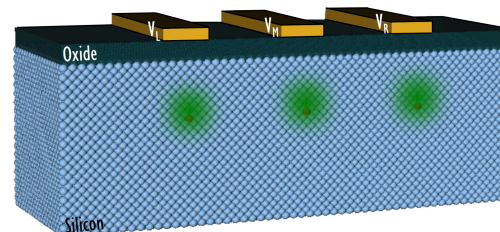
Isolated electrons

- ✓ X Rotation
- ✓ 60 MHz

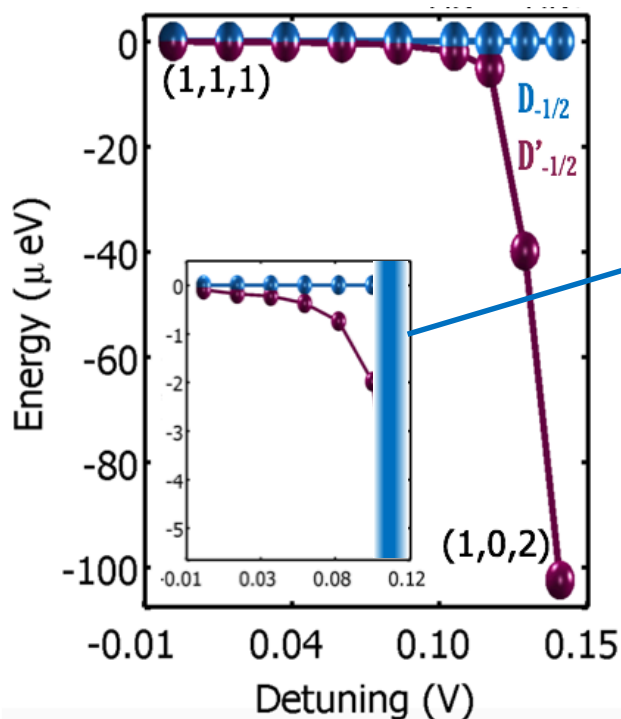


Two-axis rotations of donor based **Singlet-Triplet Qubit**

Three electron spectra from ACI
(Spin -1/2 Qubit States)



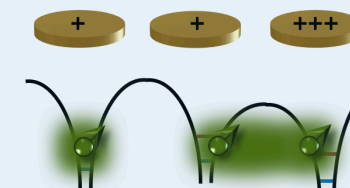
6a0 deep P donors
Separation 15nm [100]
0.1T magnetic field along Z



Qubit Manipulation

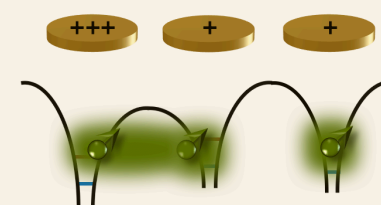
Large M-R electron exchange

- ✓ Detuning **right** donor
- ✓ 10 GHz



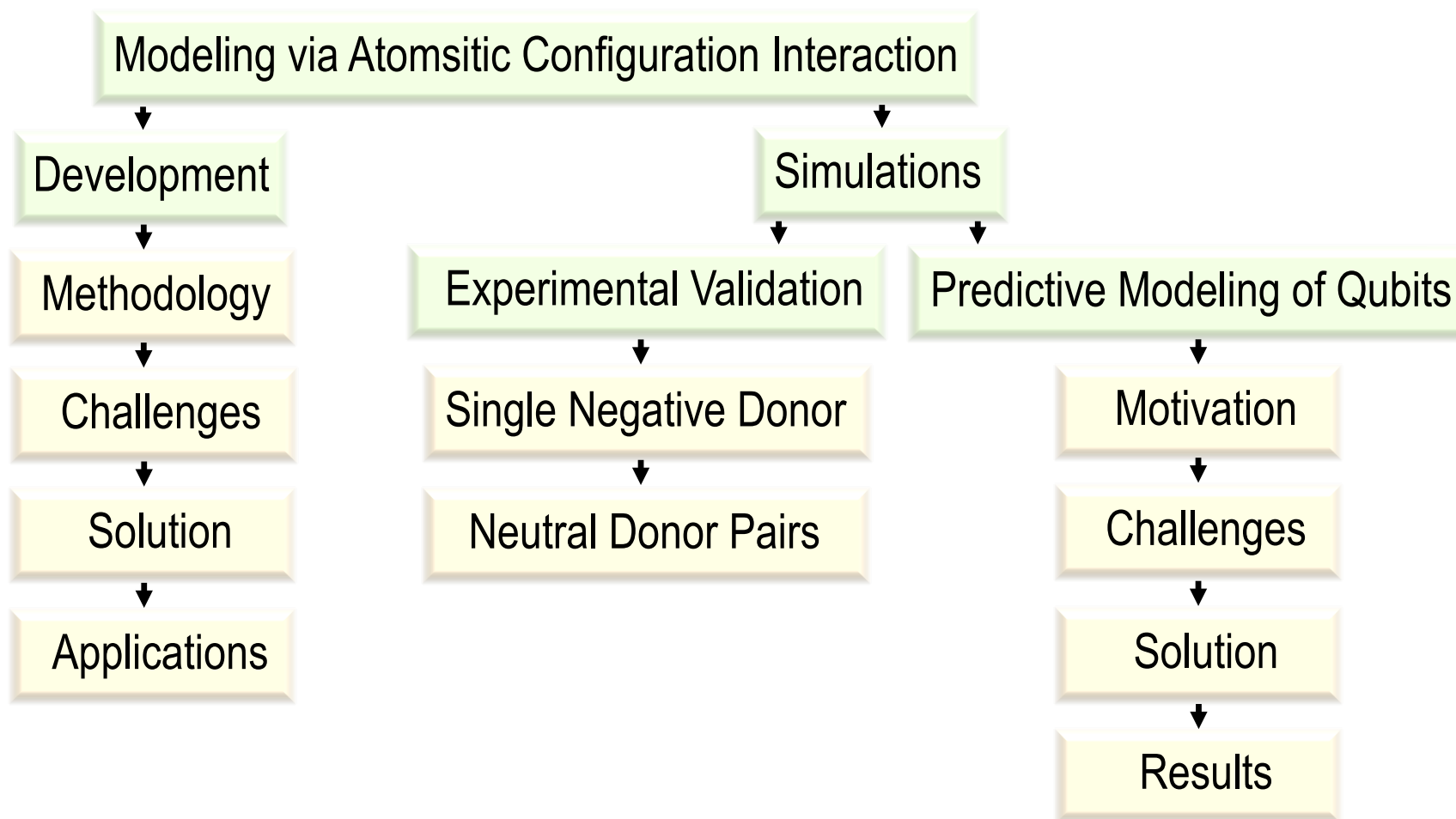
Large L-M electron exchange

- ✓ Detuning **left** donor
- ✓ Symmetric E vs. detuning
- ✓ 10 GHz



Two-axis rotations of donor based **Exchange-Only Qubit**
Isolation of qubit from leakage states

Electron Spin Qubits in Solid-State Architectures



Atomistic Configuration Interaction Tool in NEMO

- ✓ Massively parallelized and improved performance
- ✓ Large scale simulations of realistic multi-electron devices
- ✓ Validated against experimental data

Physical Insights

- ✓ For a single negative donor, second electron prefers to occupy excited states
- ✓ Approximate models to evaluate exchange in donor pairs inaccurate for large range of separations
- ✓ Exchange oscillations are suppressed for sub-surface donor pairs
- ✓ Exchange saturates for closely spaced donors in a donor pair
- ✓ Multi-spin qubits are feasible in donors without integrated micromagnets or nuclear spins

Tankasala A, Salfi J, Bocquel J, Voisin B, Usman M, Klimeck G, Simmons MY, Hollenberg LC, Rogge S, Rahman R. Two-electron states of a group V donor in silicon from atomistic full configuration interaction. arXiv preprint arXiv:1703.04175. 2017 Mar 12.

Wang Y, **Tankasala A**, Hollenberg LC, Klimeck G, Simmons MY, Rahman R. Highly tunable exchange in donor qubits in silicon. npj Quantum Information. 2016 Apr 12;2:16008.

Usman M, Bocquel J, Salfi J, Voisin B, **Tankasala A**, Rahman R, Simmons MY, Rogge S, Hollenberg LC. Spatial metrology of dopants in silicon with exact lattice site precision. Nature nanotechnology. 2016 Sep 1;11(9):763-8.

Salfi J, Voisin B, **Tankasala A**, Bocquel J, Usman M, Simmons MY, Hollenberg LC, Rahman R, Rogge S. Valley filtering and spatial maps of coupling between silicon donors and quantum dots. arXiv preprint arXiv:1706.09261. 2017 Jun 28.

Tankasala A, Ilatikhameneh H, Klimeck G, Simmons MY, Rahman R. All-electrical control of exchange based donor electron qubits in silicon. In preparation

Bocquel J, **Tankasala A**, Salfi J, Voisin B, Usman M, Klimeck G, Simmons MY, Hollenberg LC, Rahman R, Rogge S. Quantum interferences in two exchange coupled dopant atoms. In preparation

Prof. Gerhard Klimeck Prof. Rajib Rahman Prof. Sven Rogge Prof. Lloyd Hollenberg Prof. Supriyo Datta Prof. Michael Manfra



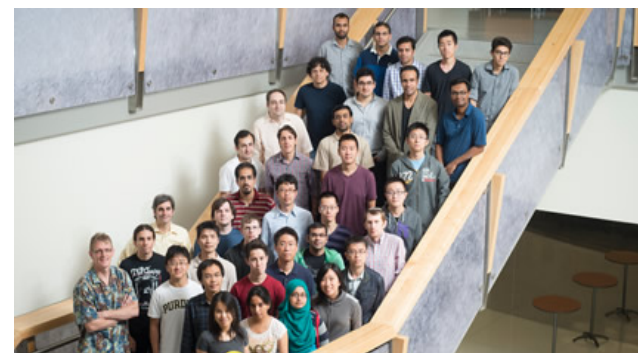
Yuling Hsueh, Rifat Ferdous, ChinYi Chen, Yu Wang, Harshad Sahasrabudhe

Dr. Juanita Bocquel, Dr. Joseph Salfi, Dr. Muhammed Usman, Dr. Benoit Voisin

Dr. Jim Fonseca, Prof. Michael Povolotskyi, Dr. Bozidar Novakovic, Dr. Jun Huang, Prof. Tillmann Kubis

Fan Chen, Hesameddin Ilatikhameneh, Tarek Ameen, Daniel Valencia, YuanChen Chu, Kuang-Chung Wang, Yui-Hong Matthias Tan, Mehdi Salmani, Kai Miao, Yaohua Tan, Junzhe Geng, Daniel Lemus, James Charles, Daniel Mejia, Prasad Sarangapani, Evan Wilson, Pengyu Long, Gustavo Valencia, Xinchun Gao, Samik Mukherjee, Enrique Aldana

Ashley Byrne, Vicki Johnson



THANK YOU !

Archana Tankasala

Q1. On slide 10, how should the hydrogenic spectrum look like? Is the energy spacing correct?

Q2. What does using shared memory model or parallelization schemes mean in terms of the hardware?

Q3. Why are multi-electron spins better? If it is because of AC electric fields instead of AC magnetic fields, what about their coherence times? What is the metric that matters for a qubit operation?

C1. “Doubly charged donor” is preferred over “Negative donor”.

C2. For a physics audience, the explanation on Hartree-Fock wavefunction can be briefer.

S1. On slide 12, it appears the second electron occupies an excited orbital state. It is confusing since the same notation is not used in slide 30.

S2. Clarify the error bars in experimental data and the reason for the J oscillations.

S3. White ellipse highlighting the two-electron spectrum is not clear. For someone looking at it for the first time, the spectrum is not very obvious.