Si DQD Modeling

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Sandia National Laboratories

Silicon Qubit Workshop, Berkeley

August 24,25, 2009

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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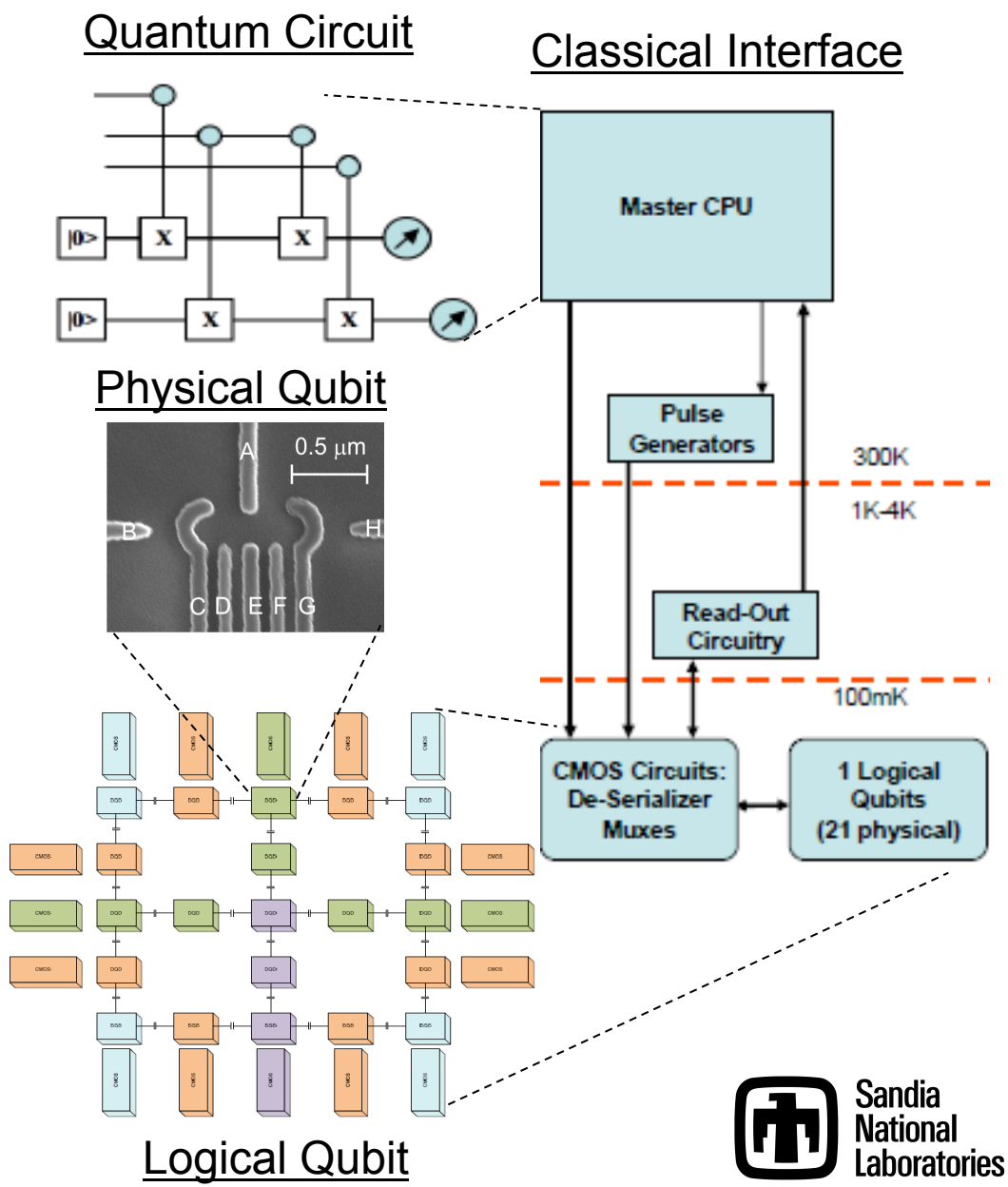
  - Mark Law (Florida)
  - Erik Nordberg (Wisconsin)
  - Harold Stalford (Oklahoma)
  - Mike Stopa (Harvard)
  - Neil Zimmerman (NIST)

Sandia DQD Effort

- Create a double quantum dot qubit using Si MOS fabrication
  - Long T2 possible
- Design a quantum circuit to perform error correction
- Focus Areas
  - Physical Qubit
  - Electronics
  - Error Correction
  - Modeling
  - Second Generation Qubit



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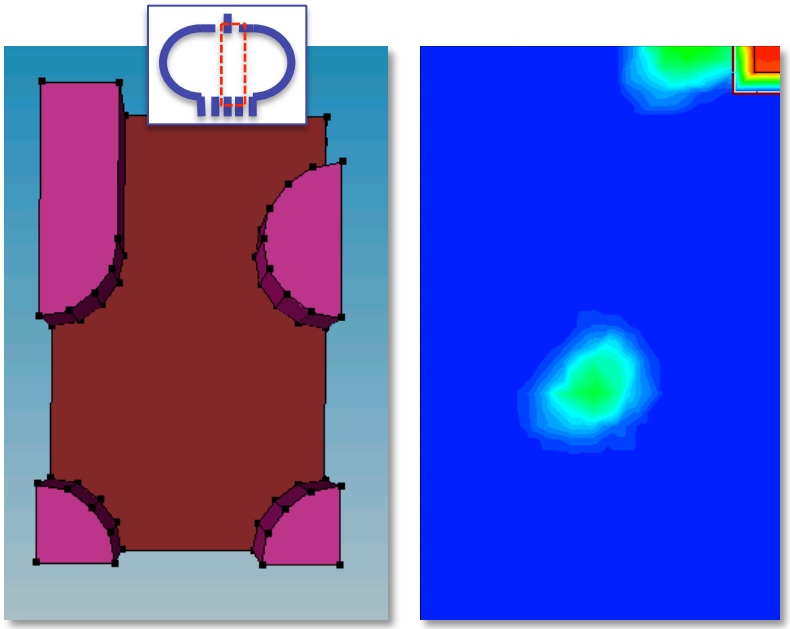
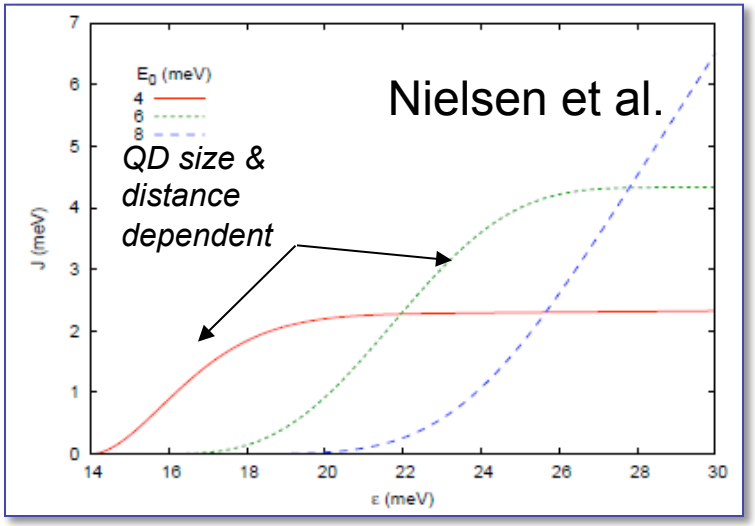
Modeling Goals

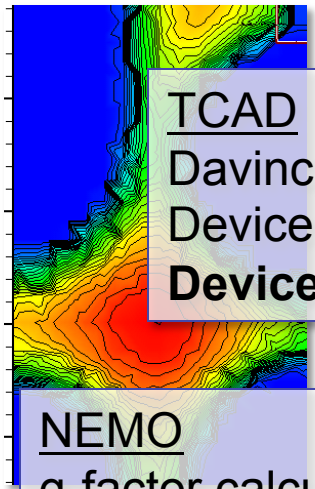
- Provide rapid guidance about device design and analysis
  - Dot size and design for few electron structures
  - Charge sensing optimization
  - Robust designs against disorder

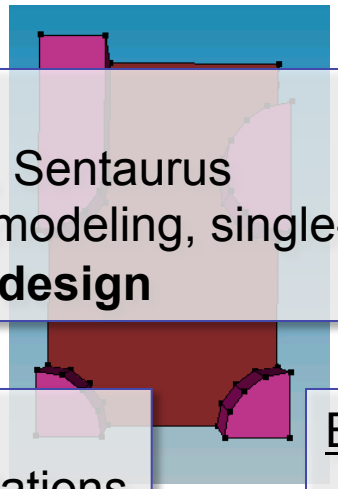
- Provide models and insight for gate performance and noise sources when experimental results are insufficient
  - Noise source identification and modeling
  - Gate design (X, Z, CPHASE)
    - Dynamic decoupling
  - Qubit transport if necessary



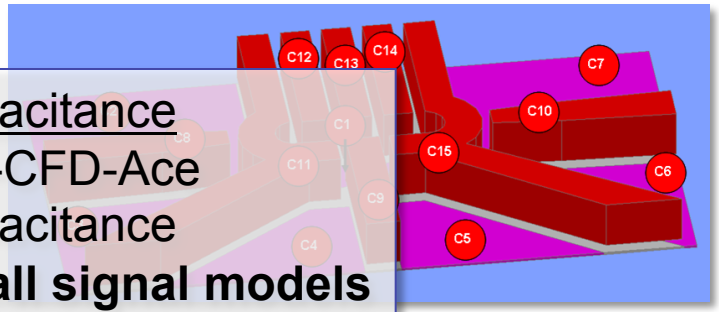


Modeling Tools

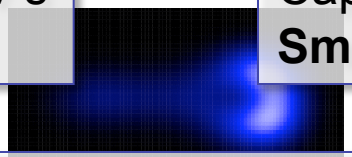




TCAD
Davinci, Sentaurus
Device modeling, single-e V's
Device design

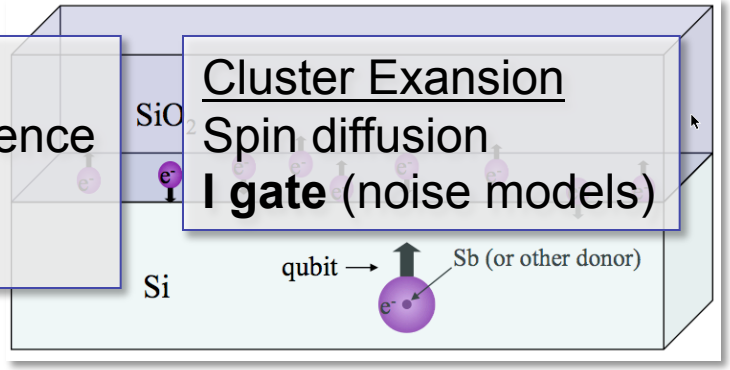


Capacitance
ESI-CFD-Ace
Capacitance
Small signal models

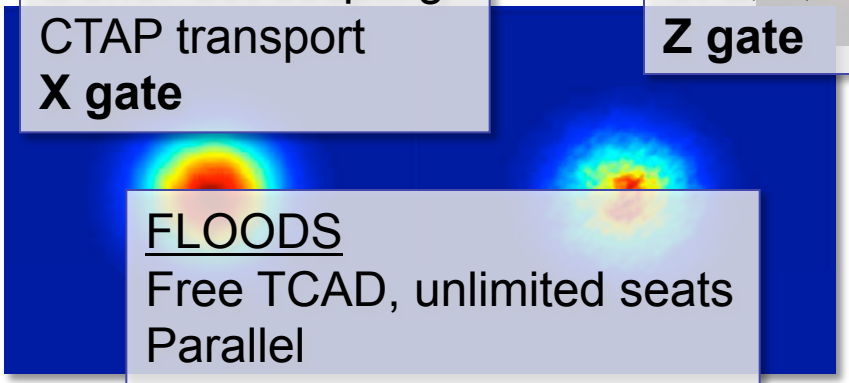


NEMO
g-factor calculations
Donor-dot coupling
CTAP transport
X gate

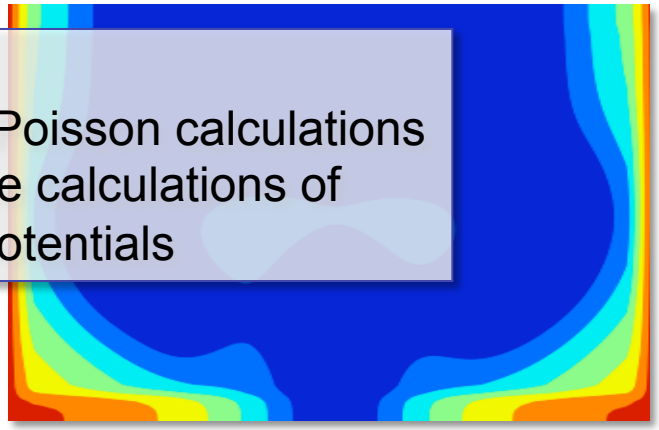
Exchange-CI
J calculations in presence of B, L, ε variations
Z gate



Cluster Exansion
Spin diffusion
I gate (noise models)



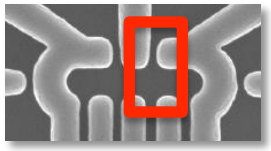
FLOODS
Free TCAD, unlimited seats
Parallel
Extend with Schrodinger-Poisson capability

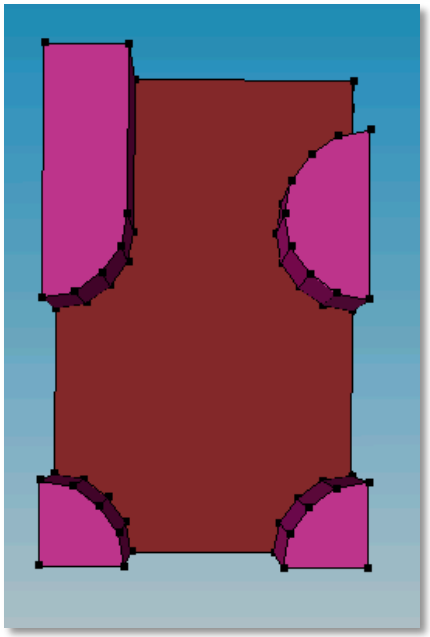


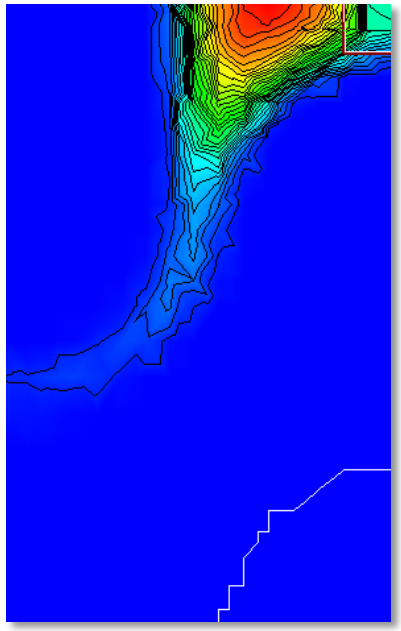
SETE
Schrodinger-Poisson calculations
More accurate calculations of double well potentials

Optimization of gate voltages

- Developed new capability to use quadratic programming to drive constrained optimization of gate parameters to target desired dot characteristics.
- Much faster than hand-optimization of gate voltages in the presence of constraints.
- Process
  - Optimize turn-on point with 1.5E11 e/cm-2 in tunnel regions (**MIT data from physical qubit team**)
  - Find gate voltages that will reduce number of electrons, keeping some parameters constant







		TGT	SIM
qd	electrons	1.0	0.9
Qdb	1e7 cm-2	1.0	0.9
Qtb	1e7 cm-2	1.0	1.0

Vag	volts		1.10
Vdbg	volts		-0.33
Vpg	volts		-1.00
Vqg	volts		0.00
Vrg	volts		-0.10

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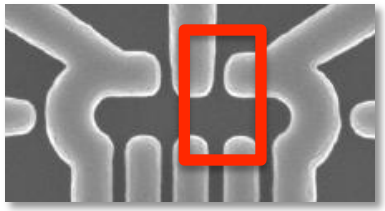
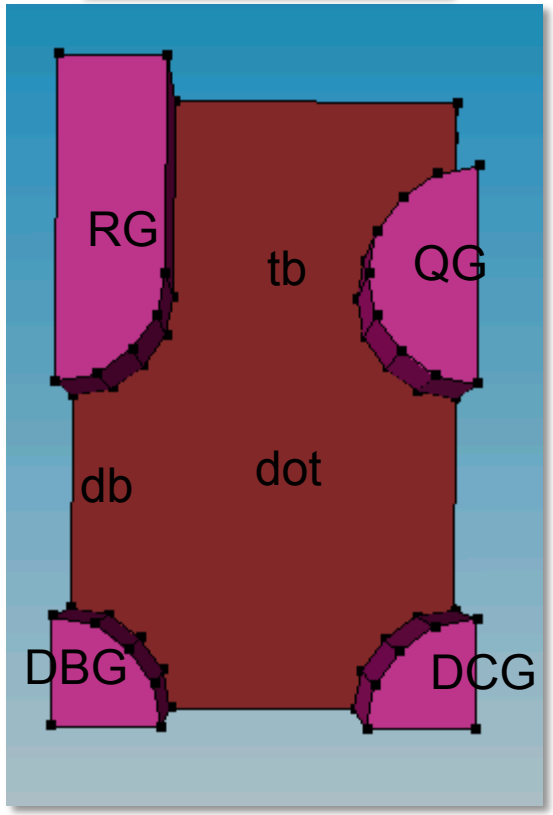
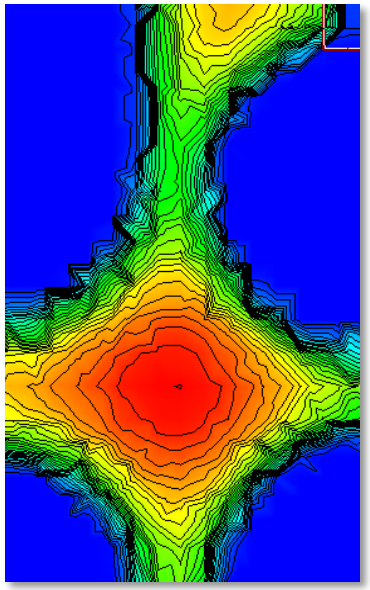
TCAD Modeling for few electrons

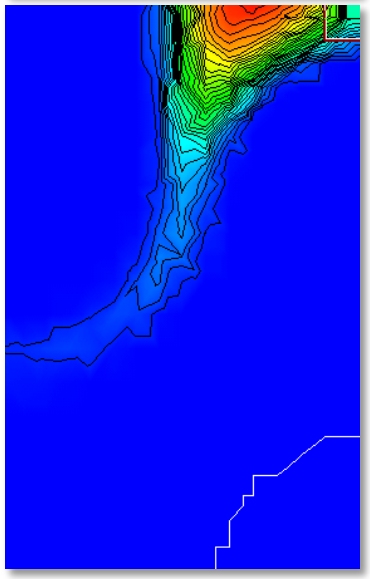




GateOxThk = 35nm
Al2O3Thk = 60nm



Qdot = 88.7 electrons
Qdb = 2.3e11 cm-2
Qtb = 1.6e11 cm-2



Qdot = 0.9 electrons
Qdb = 0.03e11 cm-2
Qtb = 0.3e11 cm-2

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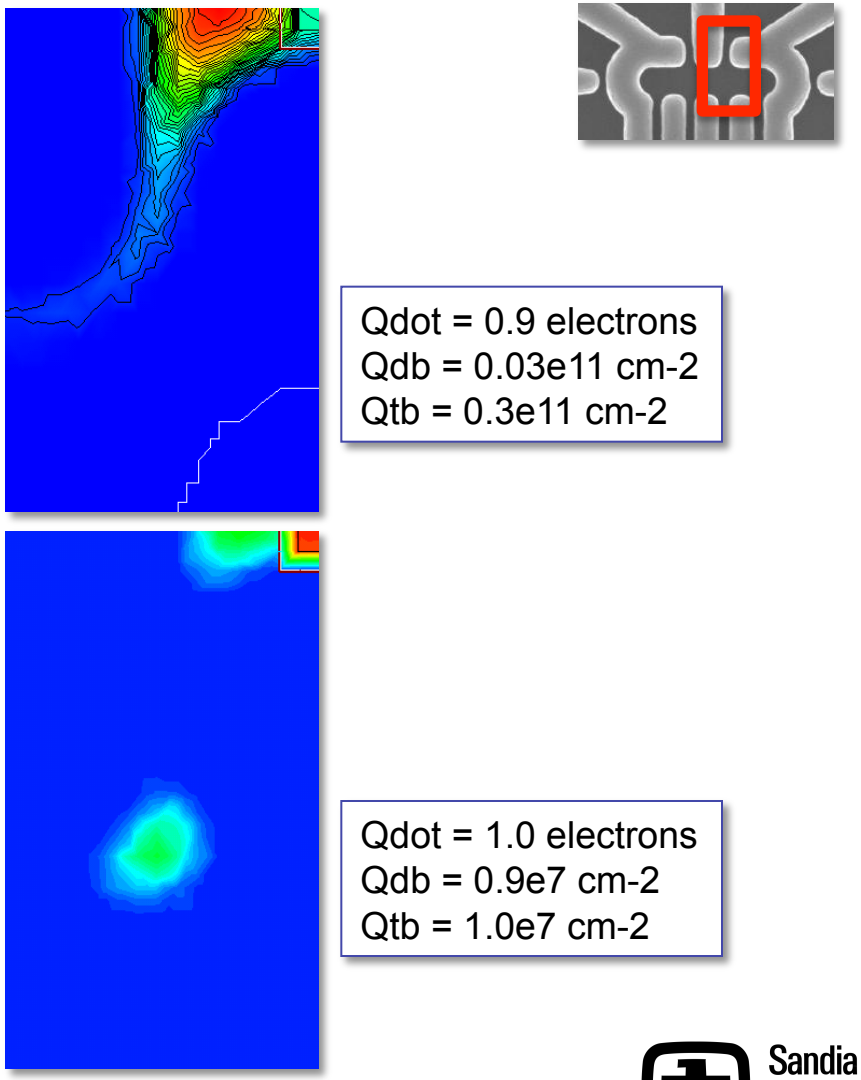
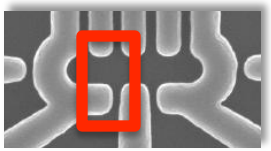
Charge sensing essential for few electrons

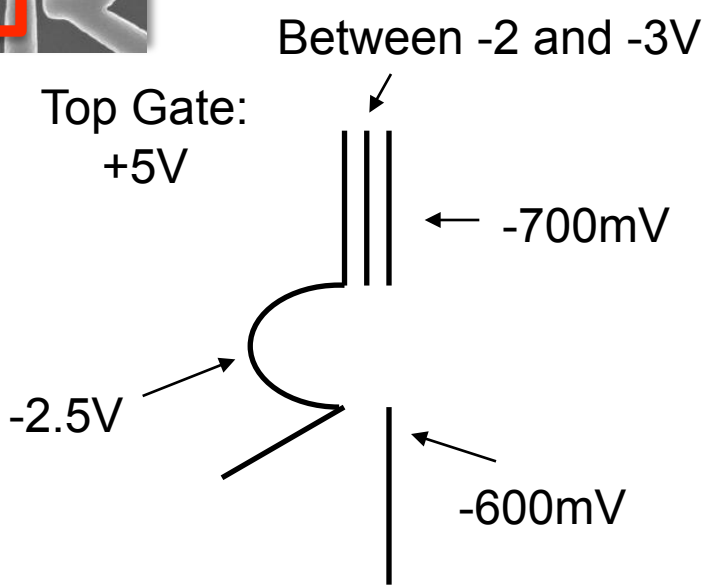
- Already experimentally recognized that charge sensing is important to obtain few-electron behavior
- Modeling has seen exactly the same problems – constraints of keeping barriers at 1.5e11 stretches dot over too wide an area
- Lowering our density in the barrier to 1e7 leads to compact dots

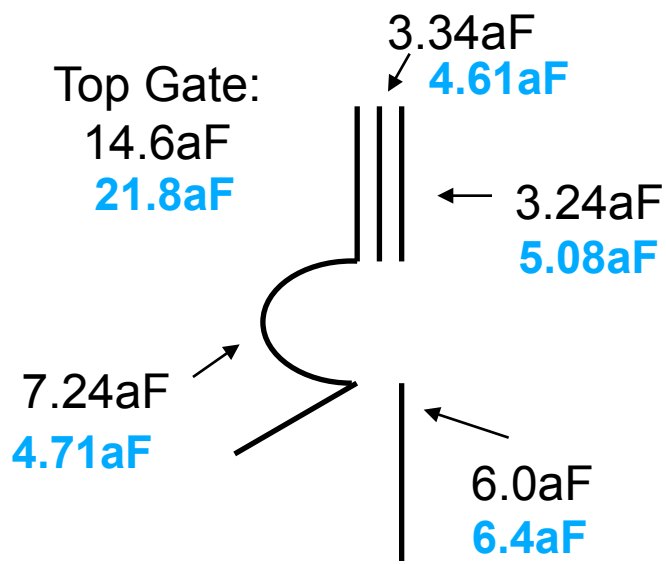


Capacitance Models in Device Sections

- Dot size from TCAD an input to capacitive network
- Can also use TCAD for capacitive checks:







Measurement
Simulation

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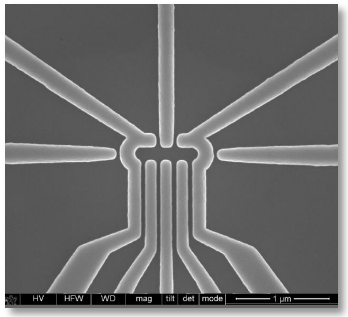
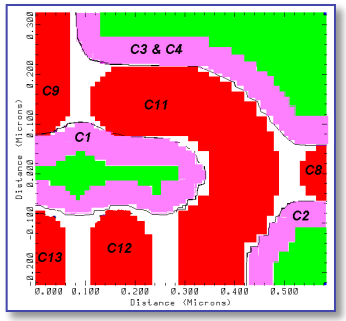
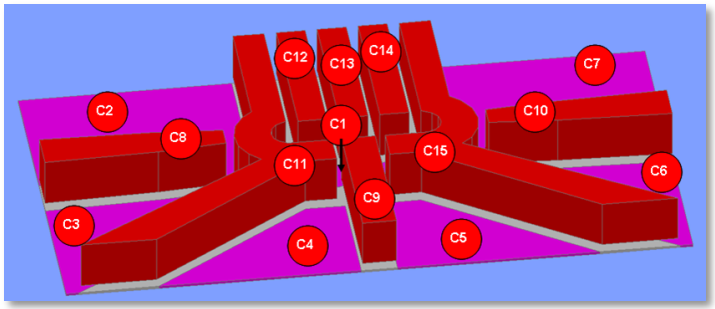
Capacitance Modeling Method

- AutoCAD Model
  - TCAD island size, density 1.5E11/ cm^2
  - Match SEM image-all dimensions
- Fabrication Process File Created
  - Describe lithography, etching, conformal deposition
- 3D Solid Model
  - Clean geometry
  - ESI's CFD-GEOM
- Capacitance Simulation
  - Meshed 3D model
  - ESI's CFD-ACE+MEMS
  - Capacitance matrix
- Scales to multiple QD simulations





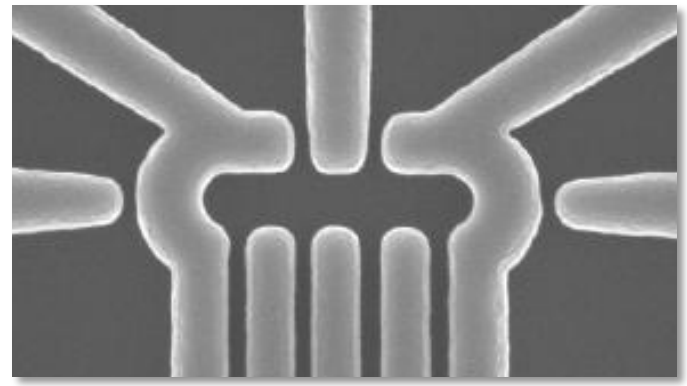


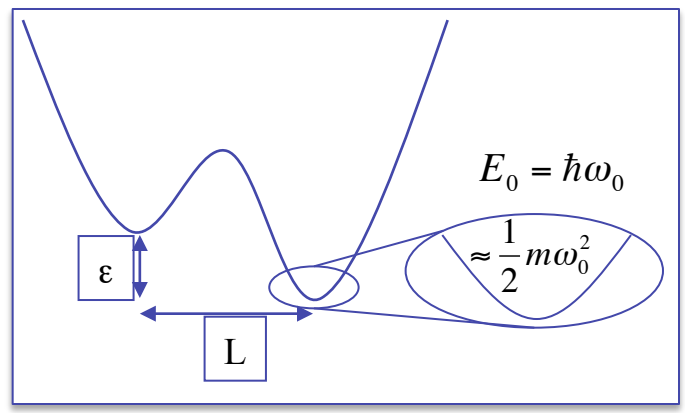
Gate	Model	Meas.
B-Q	40.2 aF	44.0 aF
C-Q	16.4 aF	14.7 aF
D-Q	16.9 aF	11.2 aF
E-Q	16.4 aF	14.1 aF
F-Q	40.2 aF	44.0 aF
H-Q	16.7 aF	20.8 aF

Z-gate Model

- Use the gate voltages to bias left, right dots to yield controlled singlet-triplet splittings, J
- The effect of the splittings yields a Z rotation

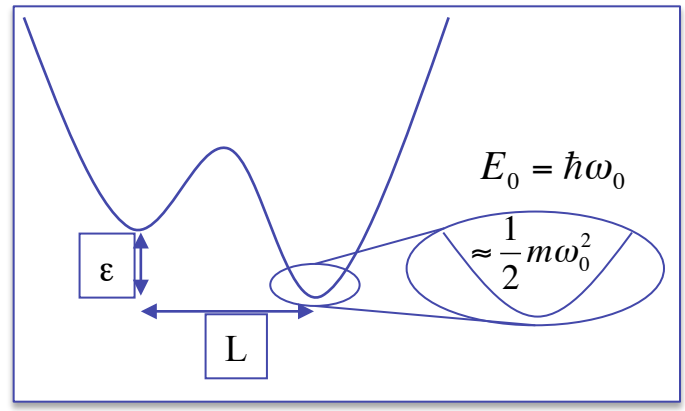
$$
\begin{aligned}
H &= \begin{pmatrix} J & 0 \\ 0 & 0 \end{pmatrix} \\
U &= e^{iHt} \cong Z(\theta = Jt)
\end{aligned}
$$



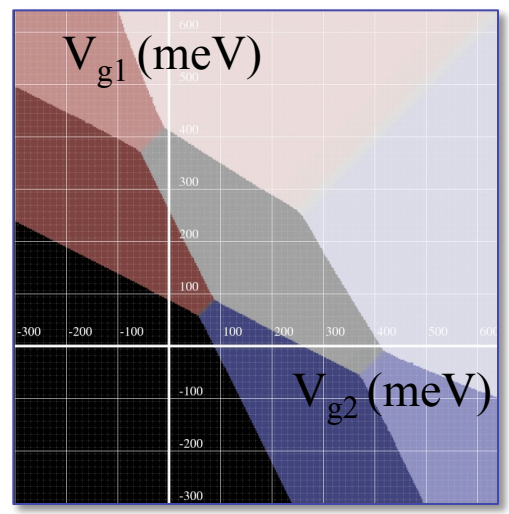


Exchange Modeling Method

- 2-electron Hamiltonian for DQD system (magnetic field perpendicular to the surface)
- Model the DQD electrostatic potential V(r) as a quartic function
- One-electron solutions expanded in gaussian basis set
- Full configuration interaction description in a (restricted) one-electron basis
- Advantages
  - Much faster than iterative Schrodinger-Poisson solvers (most Hamiltonian matrix elements can be computed analytically)
  - Can explore a greater region of parameter space (well centers at different levels)
  - Incorporation of capacitive coupling to environment allows reproduction of charge stability diagrams

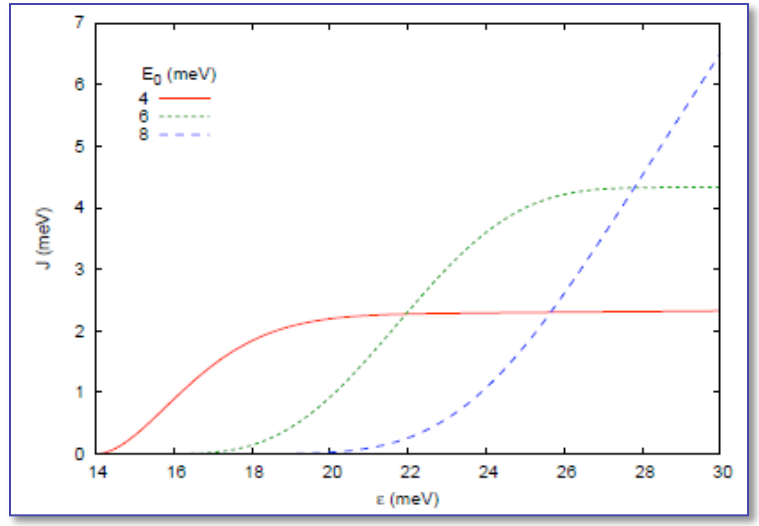


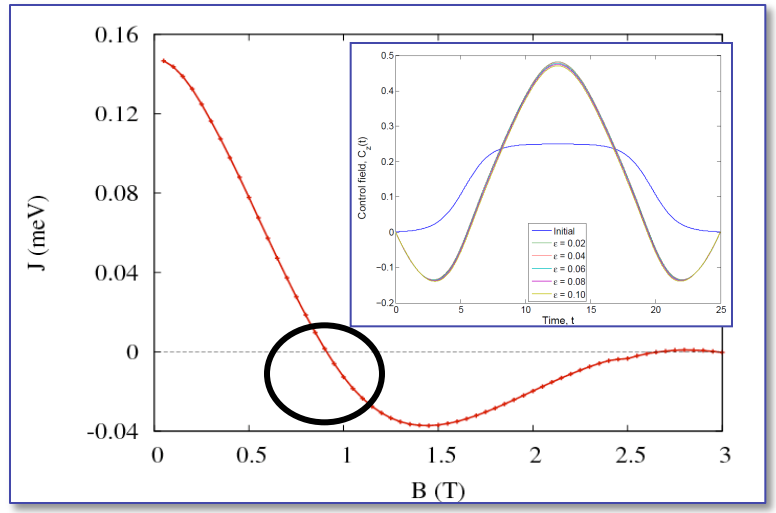
$$H = \sum_{i=1}^{2}\left[\frac{(\vec{p}_i - e\vec{A})^2}{2m} + V(\vec{r}_i) + \frac{e}{m}\vec{S}_i \cdot \vec{B}\right] + \sum_{i<j}\frac{e^2}{\kappa r_{ij}}$$



J noise, Jitter, J Flats

- Electronics limitation of pulse leads to variation in applied J
- A “plateau” region exists for ε larger than the triplet anticrossing. J is relatively constant and finite valued
- Good region for gate operation if the value of J is not too large for viable gate times.
- Plateau in J vs. ε can be lowered by increasing B, adjusting L, etc.
- By varying B, J can be tuned above and below 0. This gives additional freedom to pulse optimization



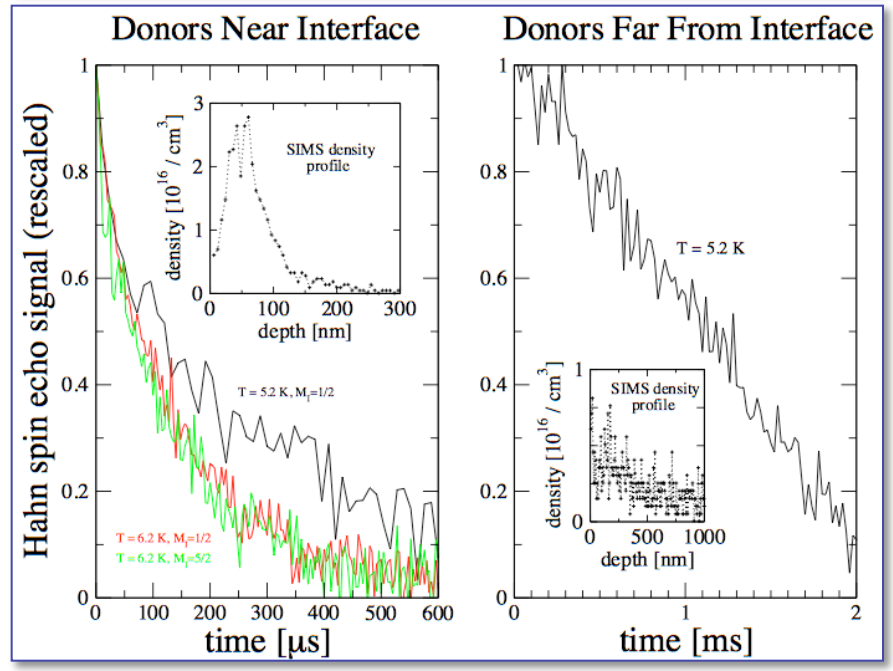


Spin Diffusion

Schenkel et al. APL

- Understand impact of P_b centers on T2 time by comparing to Schenkel's data on donor T2's at different depths
- de Sousa's model used a stochastically-driven spin **flip**, required Dit ~ 10^{14}
- Current model uses **flip-flop** model where pairs of Pb spins can exchange in concert, potentially with more realistic Dit's
- Model uses recently developed cluster expansion techniques and new variants/strategies to compute the resulting decoherence dynamics.

Sample	Interface	Peak depth (nm)	T_1 (ms)	T_2 (ms)
120 keV	Si/SiO_2	50	15±2	0.30±0.03
120 keV	Si—H	50	16±2	0.75±0.04
400 keV	Si/SiO_2	150	16±1	1.5±0.1
400 keV	Si—H	150	14±1	2.1±0.1



Cluster expansion method

- Define decoherence in terms of the evolution of the qubit density matrix in the presence of an effective Hamiltonian (flip-flop terms)
- Use cluster correlation expansion to express the decoherence in a perturbation series in size of interface spin clusters that flip-flop
- Use qubit bath perturbation techniques to accelerate convergence

$$\hat{\mathcal{H}}^{\text{eff}} = \Omega_0 \hat{S}_0^z + \Omega_1 \sum_{n\neq 0} \hat{S}_n^z + \sum_n A_n \hat{S}_0^z \hat{S}_n^z + \frac{1}{2}\sum_{n\neq m} B_{nm}(\hat{S}_n^+ \hat{S}_m^- - 2\hat{S}_n^z \hat{S}_m^z)$$

$$A_n = \gamma_e^2 \hbar \frac{1-3\cos^2\theta_{n0}}{R_{n0}^3}, \; B_{nm} = \frac{1}{2}\gamma_e^2 \hbar \frac{1-3\cos^2\theta_{nm}}{R_{nm}^3}$$

$$\frac{\rho_q^{+-}(t)}{\rho_q^{+-}(0)} \qquad \rho(t) = \hat{U}\rho(0)\hat{U}^\dagger \qquad \rho_q(t) = \mathrm{Tr}_B\, \rho(t)$$

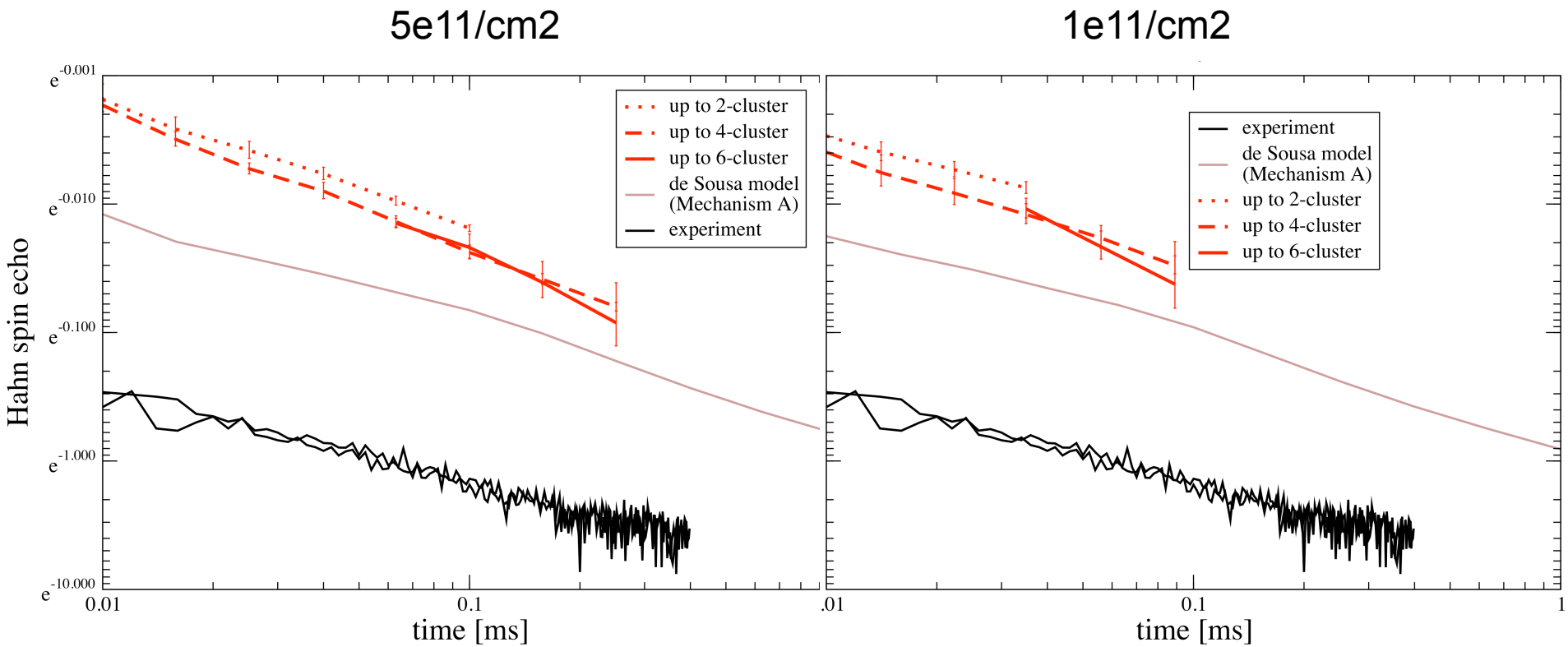
$$L^J = \langle J|\rho^{\pm}(t)|J\rangle / \rho_q^{+-}(0)$$
$$L_{\mathcal{S}}^J = \langle J|\hat{U}_{\mathcal{S}}\rho(0)\hat{U}_{\mathcal{S}}^\dagger|J\rangle / \rho_q^{+-}(0)$$

$$L^J = \prod_{\mathcal{S}} \tilde{L}_{\mathcal{S}}^J, \quad \tilde{L}_{\mathcal{S}}^J = L_{\mathcal{S}}^J / \prod_{\mathcal{C}\subset\mathcal{S}} \tilde{L}_{\mathcal{C}}^J$$

$$L_{\text{CCE}}^{(k)} = \left\langle \prod_{\|\mathcal{S}\|\leq k} \tilde{L}_{\mathcal{S}} \right\rangle_J$$

P_b induced decoherence results

Decoherence with experimental depth profile

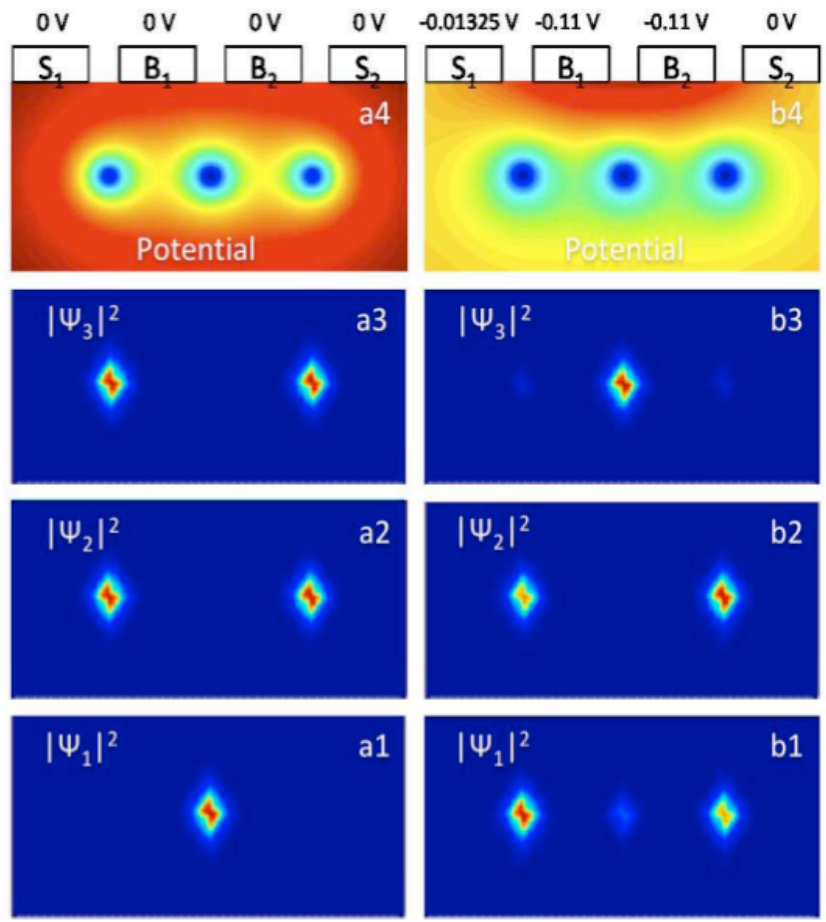


NEMO3D Modeling Capability

- All-atom tight-binding quantum mechanical simulation for micro- and nano-electronic devices
- TB program developed by Gerhard Klimeck (Purdue)
  - Ability to use high-quality basis sets for atoms ($sp^3d^5s^*$)
  - Parallelizes to 1,000's of processors
  - Ability to handle multi-million-atom calculations
  - Model a variety of phenomena under a single framework (alloy disorder, strain, TCAD potentials, interfaces, etc.)
- Code running on Sandia supercomputers
  - Test calculations have run on full 9,000 unclassified Red Storm partition
  - 3.6 M atom P in Si calculations from DQD work (11 x 60 processor jobs overnight)

CTAP + Qubit transport

- (Our initial estimates are that long-range qubit transport is not required for logical qubit.)
- CTAP is a theoretical mechanism for efficiently moving donor qubit long distances.
- NEMO3D calculations have determined adiabatic pathway for simplified case.
- Leveraging other funding for CTAP calculations.



Conclusions

- TCAD modeling effort that can give insight into V's that lead to few electron behavior
- Capacitive models that verify dot is of lithographic size, and connection to a small signal model (Harold Stalford poster)
- Exchange modeling gives predictions for Z-gate: J-flats, negative J regions
- Models of P_b induced spin decoherence (Wayne Witzel poster)
- Modeling of CTAP transfer for high fidelity qubit transport (Rajib Rahman poster)