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The QCAD Framework for Quantum Device Modeling

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LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Modeling Quantum Dots

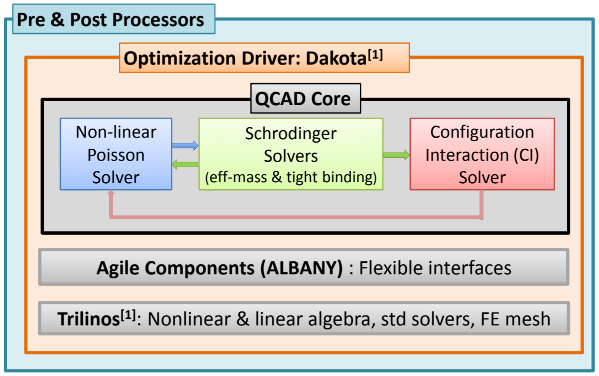
Goals

- **Design guidance**: which double quantum dot layouts perform best ?
- **Device calibration**: given a specific dot device, what gate voltages lead to few-electron behavior (threshold voltage, dot-to-gate capacitances , etc.) ?

Challenges:

- many device layouts & material stacks
- large parameter space (many gates)
- defects / disorder
- complex geometries
- low temperature

Quantum Computer Aided Design (QCAD) Device Simulator



Development Goals

- *Integration*
- *Flexibility*
- *High Throughput*

Features

- Automatic differentiation
- Evaluation order determined by graphs
- Distributed parallel computing
- All Sandia-developed!

Self-Consistent Poisson-Schrodinger (P-S)

Coupled Poisson equation:

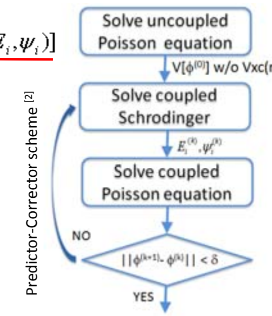
$$-\nabla(\varepsilon_s \nabla\phi) = q[p(\phi) + N_D^+(\phi) - N_A^-(\phi) - n(\phi, E_i, \psi_i)]$$

Coupled Schrodinger equation:

$$\frac{-\hbar^2}{2}\nabla\left(\frac{1}{m^*}\nabla\psi_i\right) + V(\phi,n)\psi_i = E_i\psi_i$$

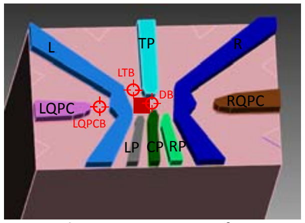
$$n(\phi, E_i, \psi_i) = \begin{cases} n(\phi) & \text{Semiclassical outside quantum region} \\ \sum_i N_i|\psi_i|^2 & \text{Quantum region} \end{cases}$$

$$V(\phi,n) = q\phi_{ref} - \chi - q\phi + V_{xc}(n)$$

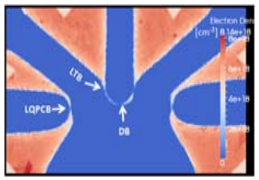


Optimization & Design Guidance

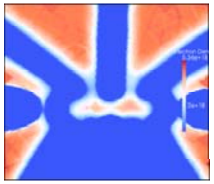
- **Dakota in conjunction with the QCAD Poisson Solver enables optimization of gate voltages for simultaneous targets**:
  - Electrons in a dot (e.g., 1e- in the left dot)
  - Electron density at a tunnel barrier automatically detected through saddle-point-searching algorithm (e.g., LTB, DB, LQPCB)
  - Distance b.t.w where a charge sensing constriction forms and where a dot forms



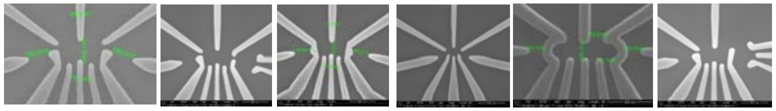
Depletion gate pattern of an experimental quantum dot



Sample 538, **1e-** in the left dot



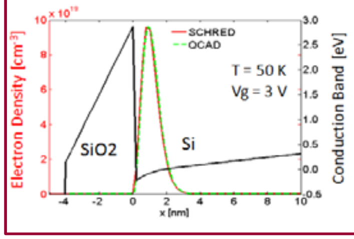
Sample 485, **100e-** in the left dot



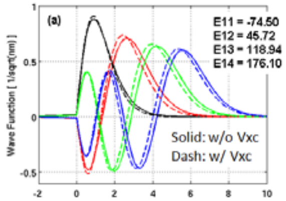
Selected SEM depletion gate patterns of experimental DQDs that have been simulated

- **What optimizations have been able to tell us :**
  - Which experimental layouts perform better (e.g., which ones allow 1e- in each dot and simultaneously turning on barriers)
  - Does barrier turn on before/after dot has many electrons? (openness)
  - Location / shape of "main" dots and charge sensing barriers/dots

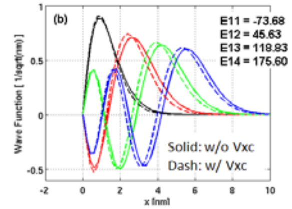
Validation of Self-Consistent P-S Solver



Wfs and energies from QCAD

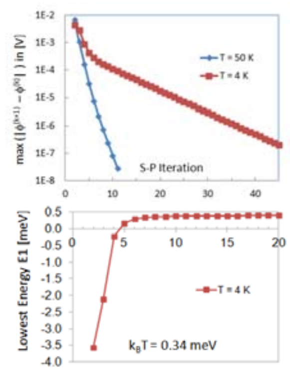


Wfs and energies from SCHRED[3]

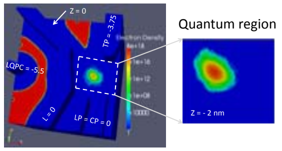


- Validate the P-S solver on a 1D MOS capacitor with 4-nm thick oxide and 5e17 cm^{-3} p-substrate doping
- Also validate the solver on a 2D gate-induced quantum wire (not shown)

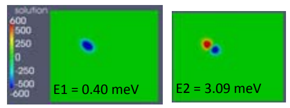
Application of Self-Consistent P-S to Quantum Dot



- Monotonic 3D P-S convergence
- More S-P iterations for low-T



Electron density at 4 K in a single dot of an experimental DQD



Lowest two wfs and energies in the z=-2 nm plane where electron density is peaked

Simulated Dot-to-Gate Capacitances

	QCAD Poisson	QCAD 3D P-S		QCAD Poisson	QCAD 3D P-S	
	T = 50 K	T = 50 K		T = 4 K	T = 4 K	
AG [V]	3.90	3.90	3.90	3.90	3.90	3.90
Q_s [x10^{11} cm^{-2}]	-4.61	-4.61	-4.51	-4.54	-4.54	-4.43
Int(n) in R_q	0.96	0.06	0.96	0.95	2.32e-19	0.95
dot-AG [aF]	3.98	1.10	4.33	4.38		4.98
dot-TP [aF]	0.33	0.07	0.37	0.37		0.44
dot-CP [aF]	0.86	0.19	0.96	0.95		1.12
dot-LP [aF]	0.64	0.14	0.72	0.71		0.84
dot-L [aF]	2.07	0.52	2.30	2.28		2.64

- For given # of e- in the dot, as T reduces, electrons stay closer to the interface, so smaller effective distance meaning higher cap.
- For given T and # of e- in the dot, quantum cap. is higher which detailed analysis shows is due to the fact that quantum charge is much broader in space, so more responsive to voltage change.

Summary

- QCAD software tool developed enables **design comparison and guidance** for semiconductor quantum dot devices.
- High throughput of simulations through scripting, automated meshing and web portal allows **fast feedback** to experiment team.
- Self-consistent quantum models in QCAD allows for **analysis of quantum effects** on device behavior (cap. etc)

[1] http://dakota.sandia.gov and http://trilinos.sandia.gov.
[2] A. Trellakis, A. T. Galick, A. Pacelli, and U. Ravaioli, J. Appl. Phys. **81**, 7880 (1997).
[3] https://nanohub.org/tools/schred.

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