

# The QCAD Framework for Quantum Device Modeling

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## Modeling Quantum Dots

### Background

- Few-/single-electron quantum dots as qubits

### Goals

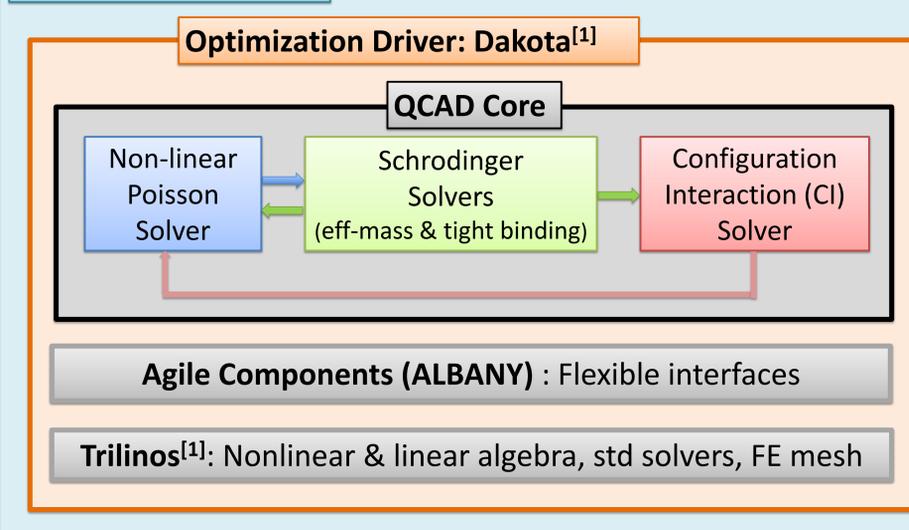
- **Design guidance:** which layouts perform best (allow few e- in each dot and simultaneous control of barriers)? given a dot device, what gate voltages lead to few-electron behavior?
- **Device calibration:** seek a systematic method of calibrating device parameters (threshold voltage, capacitance, etc.)

### Challenges

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

## Quantum Computer Aided Design (QCAD) Device Simulator

### Pre & Post Processors



### Development Goals

- Integration
- Flexibility
- High throughput
- Open source

### Features

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

## Self-Consistent Poisson-Schrodinger (P-S)

Coupled Poisson equation:

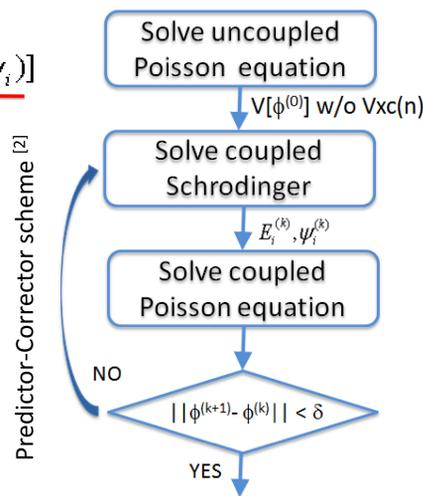
$$-\nabla \cdot (\epsilon_s \nabla \phi) = q [p(\phi) + N_D^+(\phi) - N_A^-(\phi) - n(\phi, E_i, \psi_i)]$$

Coupled Schrodinger equation:

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

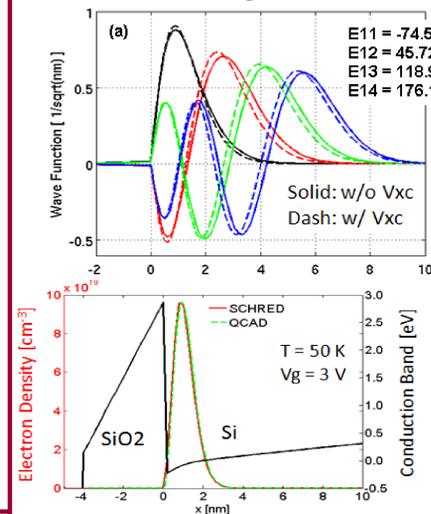
$$n(\phi, E_i, \psi_i) = \begin{cases} n(\phi) & \text{Semiclassical outside quantum region} \\ \sum_i N_i |\psi_i|^2 & \text{Quantum region} \end{cases}$$

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

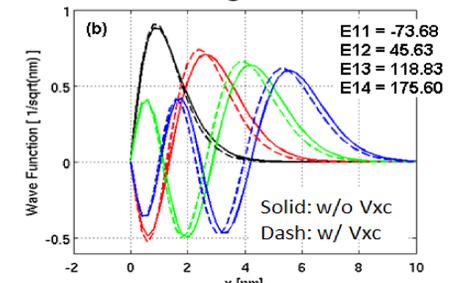


## Validation of Self-Consistent P-S Solver

Wfs and energies from QCAD



Wfs and energies from SCHRED<sup>[3]</sup>

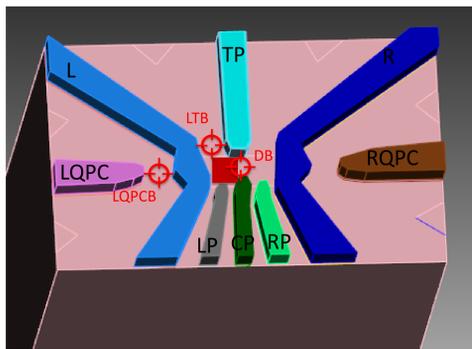


- Validate the P-S solver on a 1D MOS capacitor with 4-nm oxide and 5e17 cm<sup>-3</sup> p-substrate doping
- Also validate the solver on a 2D gate-induced quantum wire (not shown)

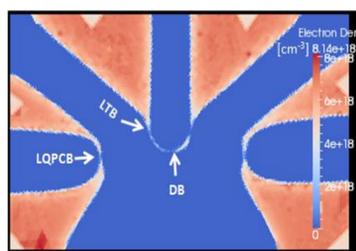
## Optimization & Design Guidance

- Dakota in conjunction with the QCAD Poisson Solver enables optimization of gate voltages for simultaneous targets:

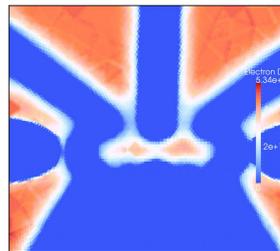
- Electrons in a dot (e.g., 1e- in the left dot)
- Electron density at a tunnel barrier automatically detected through saddle-point-searching algorithm (e.g., LTB, DB, LQPCB)
- Distance between where a charge sensing constriction forms and where a dot forms



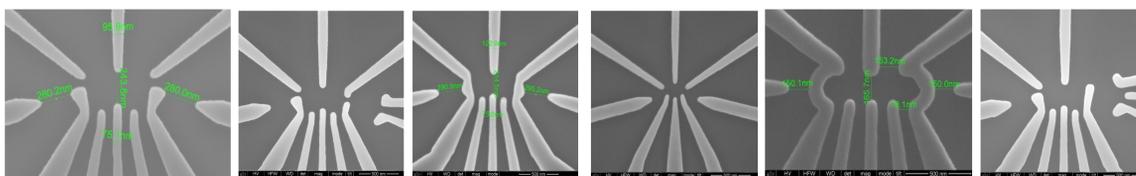
Depletion gate pattern of an experimental quantum dot



Sample A, 1e- in the left dot



Sample B, 100e- in the left dot

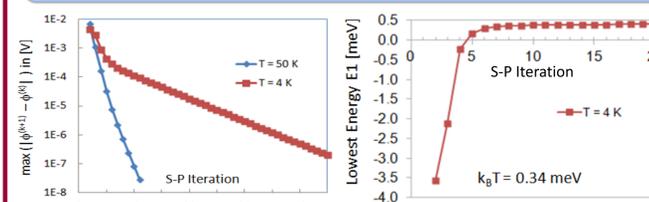


Selected SEM depletion gate patterns of experimental DQDs that have been simulated

- What optimizations have been able to tell us :

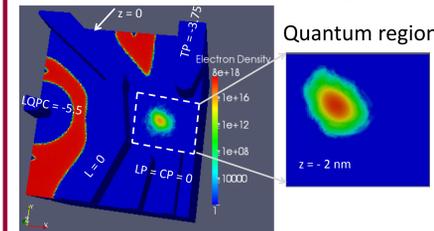
- Which experimental layouts perform better (e.g., which ones allow 1e- in each dot and simultaneously turning on barriers)
- Does barrier turn on before/after dot has many electrons? (openness)
- Location / shape of "main" dots and charge sensing barriers/dots

## Application of the P-S Solver to Quantum Dot

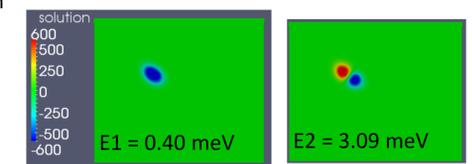


- Monotonic 3D P-S convergence
- More S-P iterations for low-T

Electron density at 4 K in a single dot



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



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
Q <sub>0</sub> [x10 <sup>11</sup> cm <sup>-2</sup> ]	-4.61	-4.61	-4.54	-4.43
Int(n) in R <sub>q</sub>	0.96	0.06	0.96	2.32e-19
dot-AG [aF]	3.98	1.10	4.33	4.98
dot-TP [aF]	0.33	0.07	0.37	0.44
dot-CP [aF]	0.86	0.19	0.96	1.12
dot-LP [aF]	0.64	0.14	0.72	0.84
dot-L [aF]	2.07	0.52	2.30	2.64

- For given # of e- in the dot, as T reduces, electrons stay closer to the interface, so smaller effective distance and higher cap.
- For given T and # of e- in the dot, quantum cap. is higher than classical one which detailed analysis reveals is because quantum charge is much broader in space, so more responsive to voltage change and higher cap.

## 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).
- Interested people can contact us about usage of the QCAD tool.

[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>.