The QCAD Framework for Quantum Device Modeling

X. Gao, E. Nielsen, R. Young, A. Salinger, R. P. Muller
Sandia National Laboratories,
1515 Eubank SE, Albuquerque, NM 87123, USA
e-mail: xngao@sandia.gov

Semiconductor quantum dot devices for quantum information processing have shown remarkable progress [1] in recent years. Sandia National Laboratories [2] has been involved in an effort to demonstrate a Si-based quantum dot qubit for quantum computing. A physics-based robust tool capable of quantum device modeling is vital to facilitate the experimental development of this technology. The Sandia Quantum Computer Aided Design (QCAD) project is developing an integrated tool to analyze and advance designs of quantum dots used as qubits, targeting the specific issues involved in few-electron, very-low-temperature dot devices, and leveraging a number of existing Sandia cutting-edge software packages [3], including the Trilinos nonlinear and linear solvers library, the Albany/Agile tool chain, the Dakota optimization toolbox, and the Cubit mesher.

As a first step, we have developed a semiclassical nonlinear Poisson solver, including Maxwell-Boltzmann (MB) and Fermi-Dirac (FD) statistics and incomplete ionization of dopants at low temperatures, which provides a good first-order description of the electrostatics in quantum devices.

One unique component of our QCAD framework includes an interface to a robust optimizer, Dakota [3], which, in conjunction with the Poisson solver, can find gate voltages that are likely to lead to few-electron quantum dots. Fig. 1(a) shows a top view of the polysilicon depletion gate pattern (transferred from SEM image) in an experimental Si quantum dot. Fig. 1(b) shows a top view of the electron density at T = 0.2 K in silicon at the Si/SiO2 interface of one optimization scenario, where the depletion gates (TP, CP, LP tied to RP, L tied to R, LQPC tied to RQPC) and top Aluminum gate AG (not shown) voltages are allowed to vary, so as to obtain one electron (integrated electron density close to one) in the left dot and simultaneously turn on the left tunnel barrier (LTB in the figure), dot barrier (DB), and left QPC barrier (LQPCB). The gate voltages that meet these optimization targets are given in the caption of Fig.1.

In addition to the semiclassical Poisson solver, we have developed a self-consistent Poisson-Schrodinger (P-S) solver in QCAD to capture quantum effects in nanostructures. The P-S capability solves the effective mass Schrodinger equation, including exchange-correlation effects, using the local density approximation [4]. Efficient convergence of the self-consistent solution is achieved utilizing a predictor-corrector iteration scheme [5]. The P-S solver currently solves the conduction Δ_2-valleys in silicon devices (whose principle axis is perpendicular to the Si/SiO2 interface) due to their lower energy and the targeted low-T applications.

Fig.2 compares the Δ_2-valley lowest four wave functions and energies in a 1D MOS capacitor between QCAD and SCHRED [6]. The results produced by the two tools show excellent agreement. Fig.3 shows the electron density and wave functions in a Si quantum dot obtained from the self-consistent P-S solver. These self-consistent 3D results are preliminary at this stage and we intend to perform extensive self-consistent simulations of realistic quantum dots and compute capacitances to compare with experimental data.

In summary, we have described the development of the QCAD program that has become a versatile tool for simulating multi-dimensional quantum devices. QCAD simulations of realistic quantum dots allow fast and valuable

feedback to accelerate the experimental development of few-electron quantum dots at Sandia.

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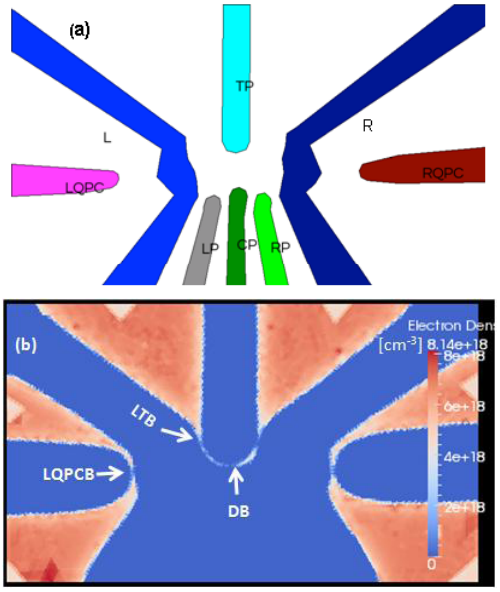
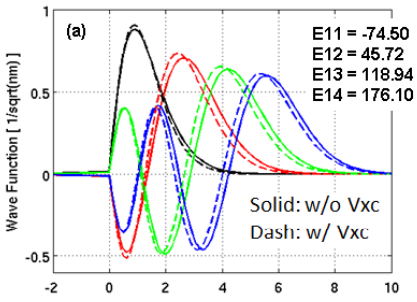


Fig.1. (a) Top view of the depletion gate pattern in a 3D Si quantum dot. (b) Top view of electron density at the Si/SiO2 interface and T = 0.2 K. The gate voltages that meet the optimization targets are AG = 3.48 V, TP = -0.74 V, CP = -0.007 V, LP = RP = -5.95 V, L = R = -1.15 V, LQPC = RQPC = -2.41 V.



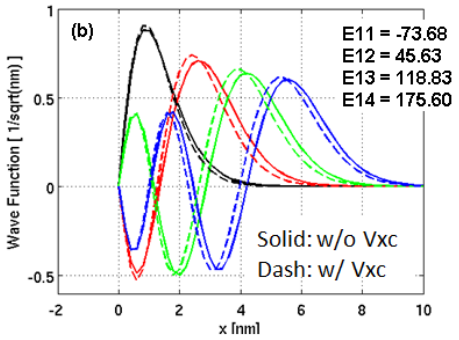


Fig.2. Δ_2-valley lowest four subband wave functions and energies in a 1D MOS capacitor with 4-nm thick oxide and 5e17 cm^{-3} p-type substrate doping at T = 50 K and Vg = 3 V obtained from QCAD (a) and from SCHRED (b). The solid and dashed curves are obtained without and with the exchange-correlation effect, respectively. Also shown are the subband energies in [meV] (referred to Fermi level) with the exchange-correlation effect. The wave functions and energies between QCAD and SCHRED show excellent agreement.

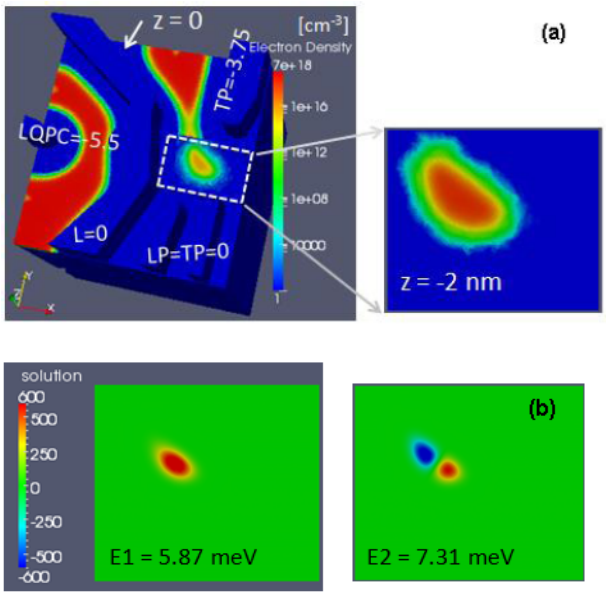


Fig.3. (a) Electron density in an experimental Si quantum dot device at T = 50 K obtained from the self-consistent Poisson-Schrodinger solver. The indicated voltages are experiment operating values. The z = 0 surface is the Si/SiO2 interface where the interface charge is used as a tuning parameter to obtain integrated electron density equal to one. The dash white box denotes the quantum region where the self-consistent solver is applied and the semiclassical Poisson solver is used in the rest of the device. Also shown is the electron density in the z = -2 nm surface where it shows peak values. (b) The lowest two wave functions in the quantum region at the z = -2 nm surface.