SAND2011-9453C

LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Semiclassical Poisson and Self-Consistent Poisson-Schrodinger Solvers in QCAD

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National Nuclear Security Administration

U.S. DEPARTMENT OF ENERGY

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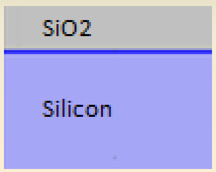
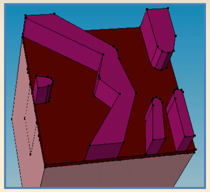
Outline

Poisson Solver Background

$$-\nabla(\varepsilon_s \nabla \phi) = q(p - n + N_D^+ - N_A^-)$$

Applications of Poisson Solver

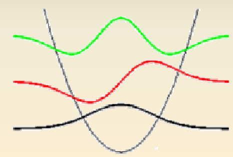


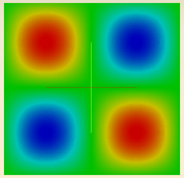


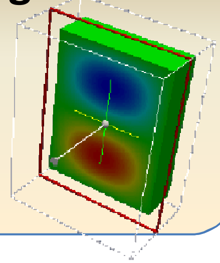
Schrodinger Solver

$$-\frac{\hbar^2}{2}\nabla\left(\frac{1}{m^*}\nabla\psi\right) + V\psi = E\psi$$

Applications of Schrodinger Solver

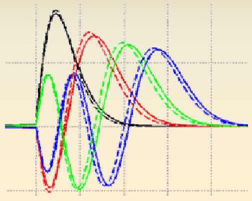


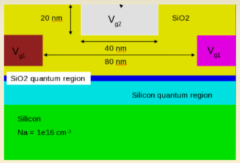


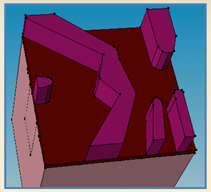


Self-Consistent Poisson-Schrodinger Solver

Applications of Self-Consistent P-S Solver







Poisson Solver – Carrier Statistics

Poisson equation in a semiconductor: $-\nabla(\varepsilon_s \nabla \phi) = q\underbrace{(p - n + N_D^+ - N_A^-)}_{f(\phi)\,=\,?}$

Maxwell-Boltzmann (MB) statistics

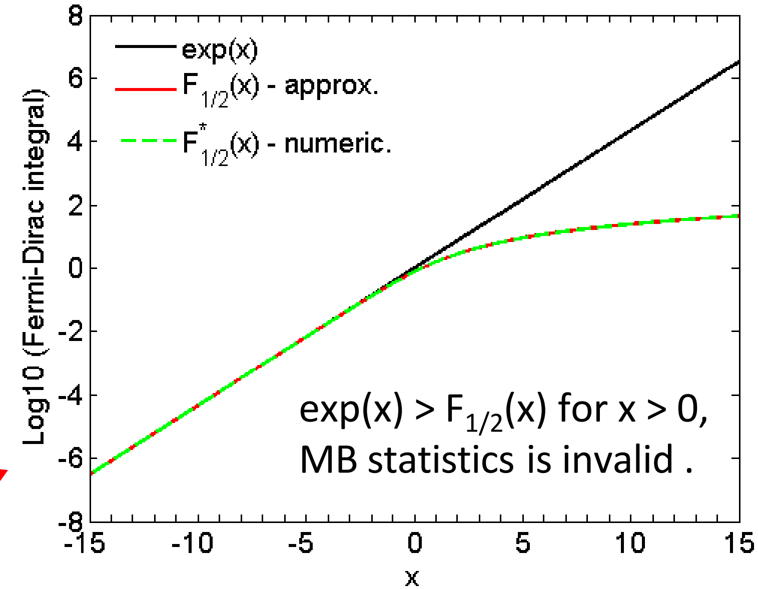
$$n = N_C \exp\left(\frac{E_F - E_C}{k_B T}\right) \qquad p = N_V \exp\left(\frac{E_V - E_F}{k_B T}\right)$$

Fermi-Dirac (FD) statistics

$$n = N_C F_{1/2}\left(\frac{E_F - E_C}{k_B T}\right) \qquad p = N_V F_{1/2}\left(\frac{E_V - E_F}{k_B T}\right)$$

Fermi-Dirac integral of 1/2 order

$$F_{1/2}(x) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{\varepsilon}\, d\varepsilon}{1 + \exp(\varepsilon - x)}$$



Approx. $F_{1/2}(x) = \left(e^{-x} + \frac{3\sqrt{\pi}}{4}\nu^{-3/8}\right)^{-1}$ [1]

$$\nu = x^4 + 50 + 33.6x\{1 - 0.68\exp[-0.17(x+1)^2]\}$$

[1] J.S. Blakemore, Solid-State Electron., Vol. 25, pp. 1067-1076, 1982.

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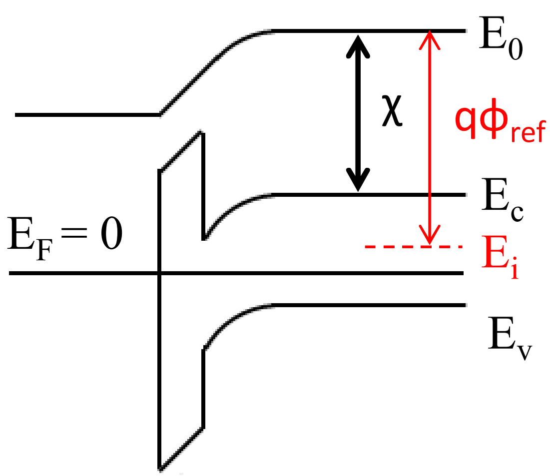
Poisson Solver – What Solved

Under thermal equilibrium (No current flow), $\mathbf{E_F}$ **= const** through out a device, chosen to be 0 in QCAD.



$$E_c = -q(\phi - \phi_{ref}) - \chi$$
$$E_v = -q(\phi - \phi_{ref}) - \chi - E_g$$

$$n(\phi)\ ,\ p(\phi)$$

Heterostructure:

- E_c & E_v are discontinuous
- Vacuum level E_0 is continuous

Requirement of potential (ϕ):

- Continuous everywhere

Choice of potential (ϕ):

- Let $-q(\phi - \phi_{ref}) = E_0 = E_c + \chi$

Constant shift

Choice of $q\phi_{ref}$ does not change the E_c and E_v profiles, but could lead to different numerical behavior during simulation.

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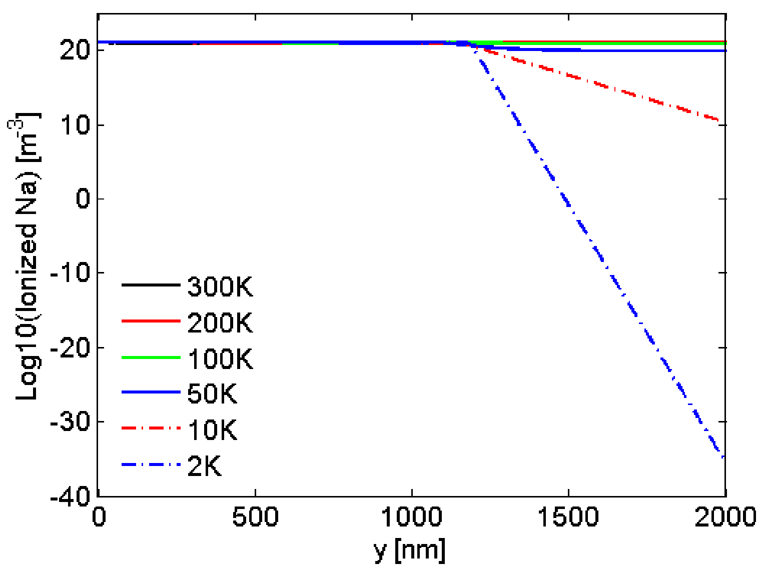
Poisson Solver – Incomplete Ionization

$$-\nabla(\varepsilon_s \nabla \phi) = q(p - n + N_D^+ - N_A^-)$$

$$\boxed{N_D^+ = \frac{N_D}{1 + 2\exp\left(\frac{E_F - E_D}{k_B T}\right)}} \qquad \boxed{N_A^- = \frac{N_A}{1 + 4\exp\left(\frac{E_A - E_F}{k_B T}\right)}}$$

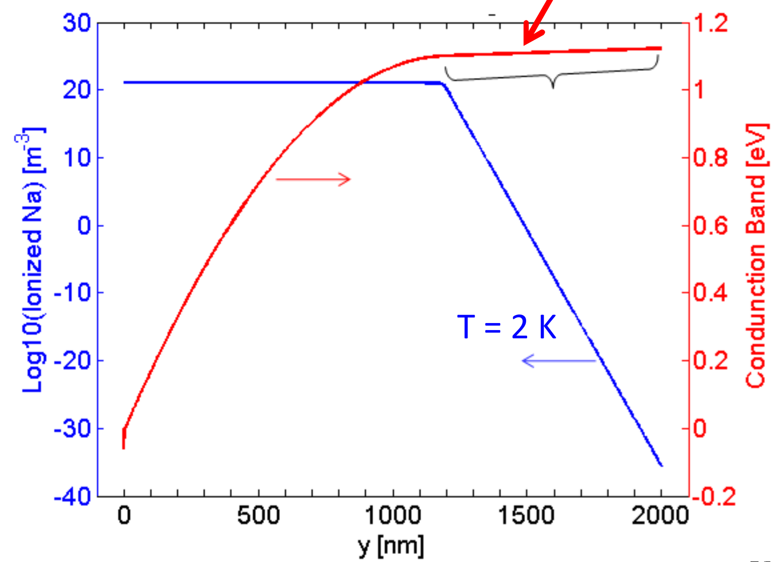
Follow Fermi-Dirac distribution

$N_{A,D}$ = dopant concentration, $E_{A,D}$ = dopant activation energy level



Significant incomplete ionization for T <= 10 K

No charge neutral region, behave like insulator (no carriers)



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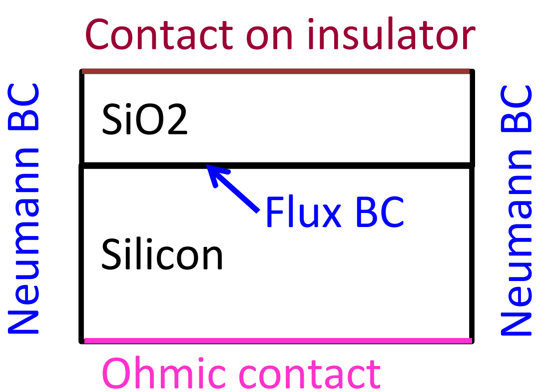
Poisson Solver – Boundary Condition

Three types of boundary conditions:

- Flux conservation b.t.w. different materials: $\varepsilon_{s1}\nabla\phi_1 \bullet \hat{\eta}_1 = \varepsilon_{s2}\nabla\phi_2 \bullet \hat{\eta}_2$
- Neumann condition: $\varepsilon_s \nabla\phi \bullet \hat{\eta} = 0$

Automatically satisfied in the finite element framework

- Dirichlet condition: $\phi = const$
  - Contact on insulator
  - Ohmic contact



Contact on insulator:

$$\phi_{ins} = V_g - (\Phi_M - q\phi_{ref})/q$$

Ohmic contact:

charge neutrality and equilibrium conditions hold

$$n(\phi) + N_A^-(\phi) = p(\phi) + N_D^+(\phi)$$

Example: p-type sc with MB at 300 K,

$$\phi_{ohmic} = V_a - \frac{k_B T}{q}\ln\left(\frac{N_A}{n_i}\right)$$

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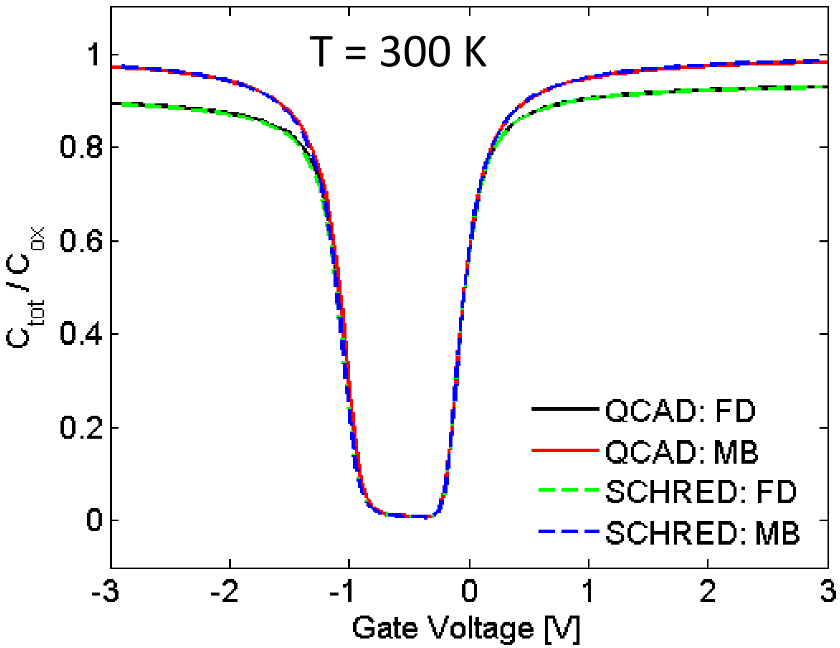
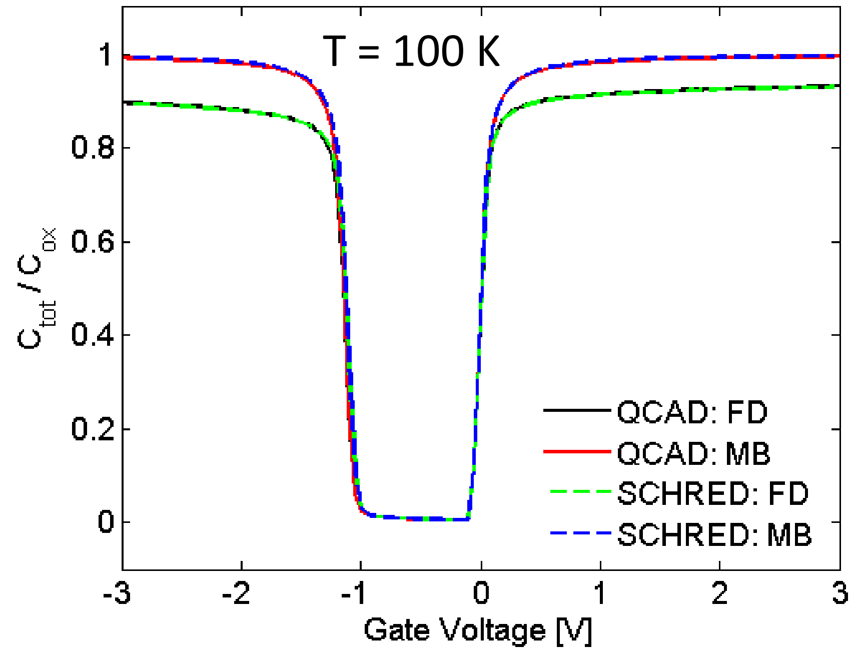
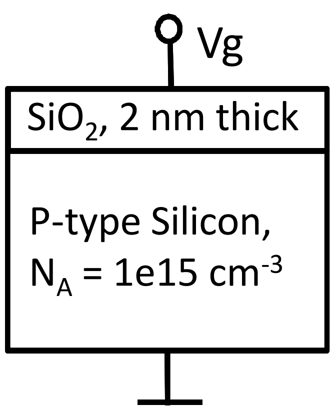
Poisson Solver – Application 2D

Apply the Poisson solver to simulate a PMOS capacitor



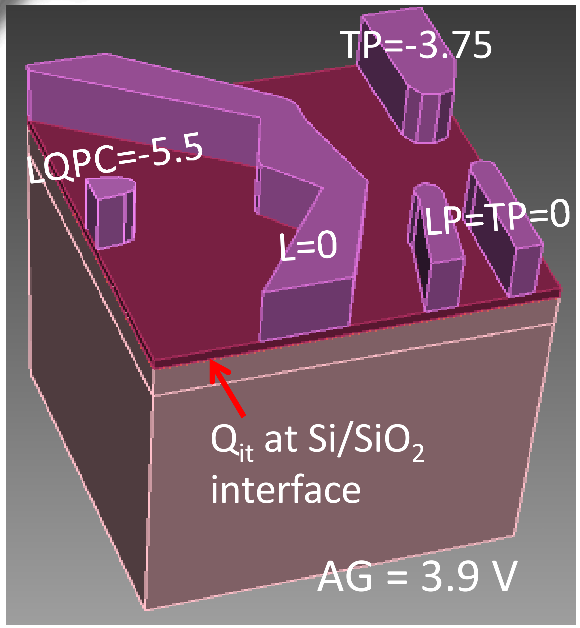




The agreement between QCAD and SCHRED validates the accuracy of QCAD Poisson solver.

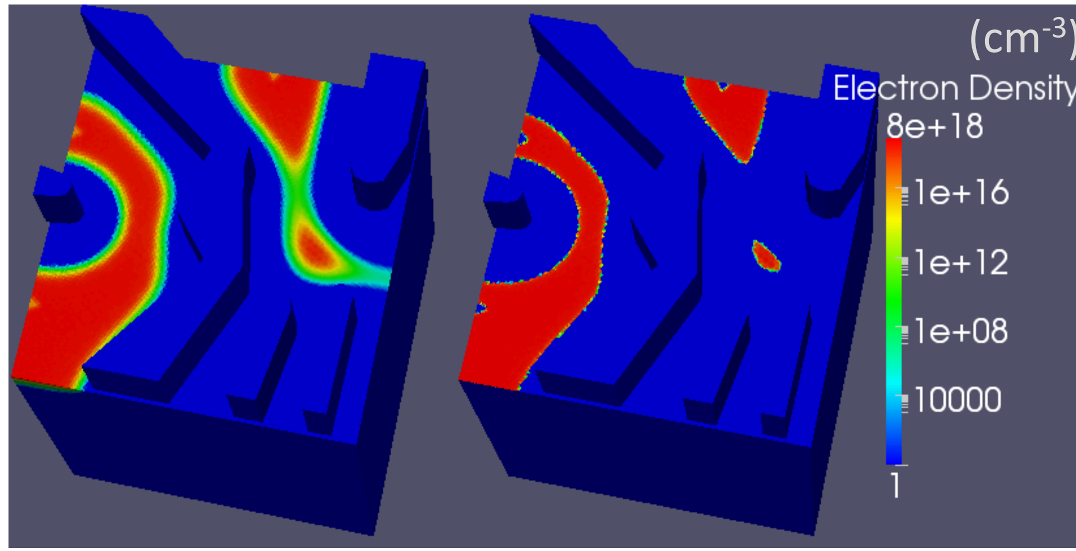
[2] https://nanohub.org/tools/schred

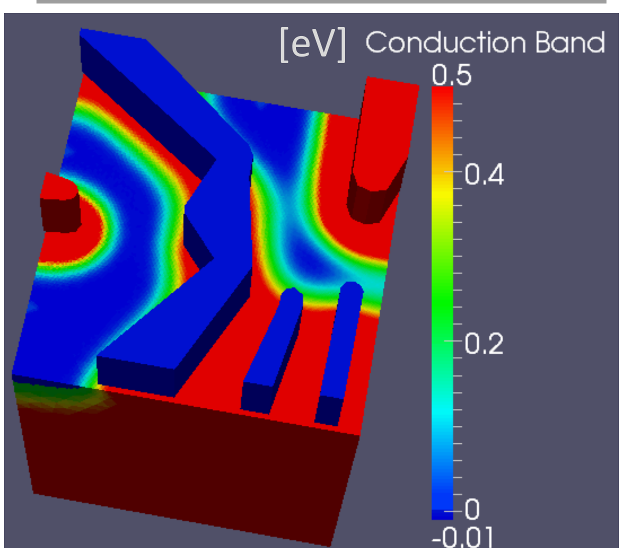
Poisson Solver – Application 3D



T = 50 K
Q_{it} = -6.235x10^{11} cm^{-2}

T = 2 K
Q_{it} = -6.16x10^{11} cm^{-2}

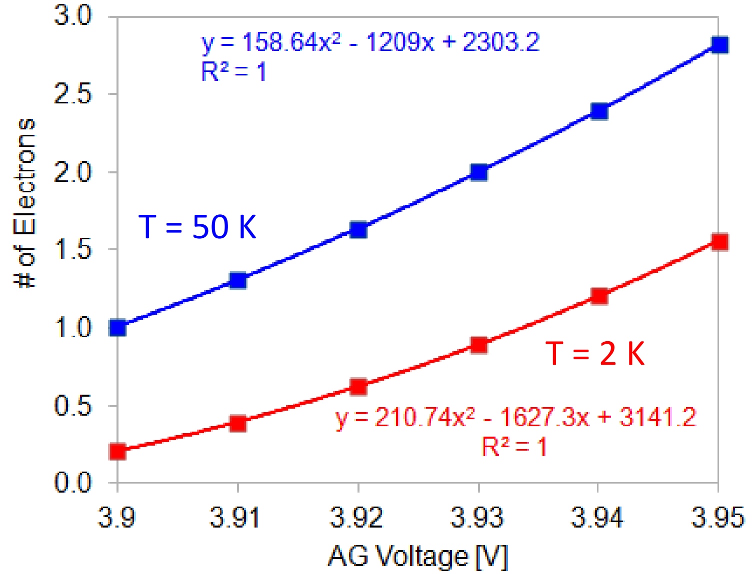




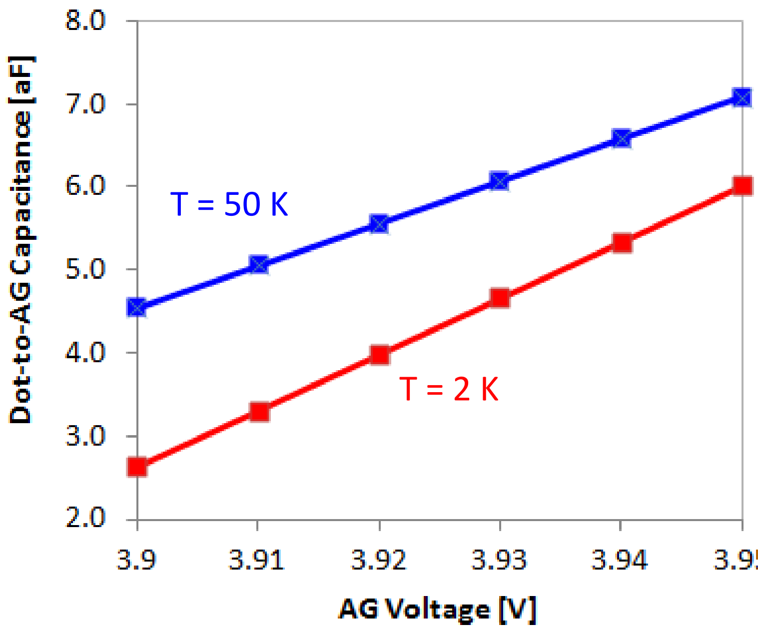
	Exp.	QCAD T = 50 K	QCAD T = 2 K	QCAD T = 2 K
Q_{it} [cm^{-2}]	?	-6.235x10^{11}	-6.16x10^{11}	-6.235x10^{11}
# of e	1	1.009	0.997	0.21
AG [aF]	2.37	4.765	5.29	2.97
TP [aF]	0.48	0.315	0.35	0.18
CP [aF]	0.54	0.778	0.857	0.63
LP [aF]	0.29	0.582	0.642	0.52
L [aF]	0.56	1.91	2.11	1.30

Poisson Solver – Application 3D

Q_{it} = -6.235 x 10^{11} cm^{-2}	T = 50 K	T = 2 K
Ramp AG	# of e in dot	# of e in dot
3.9	1.0090	0.2097
3.91	1.3064	0.3954
3.92	1.6383	0.6232
3.93	2.0026	0.8935
3.94	2.3977	1.2081
3.95	2.8222	1.5604



Q_{it} = -6.235 x 10^{11} cm^{-2}	T = 50 K	T = 2 K
Ramp AG	C_{dot-AG} [aF]	C_{dot-AG} [aF]
3.9	4.5484	2.6388
3.91	5.0567	3.3140
3.92	5.5650	3.9892
3.93	6.0732	4.6644
3.94	6.5815	5.3397
3.95	7.0898	6.0149



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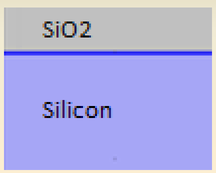

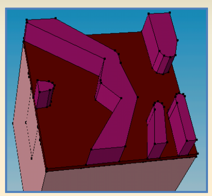

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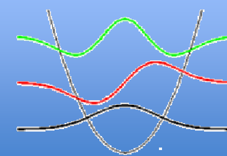
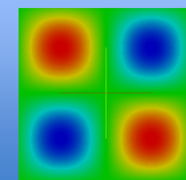
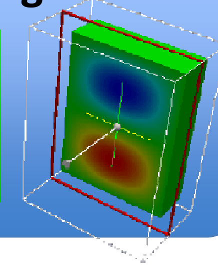
$$-\frac{\hbar^2}{2}\nabla\left(\frac{1}{m^*}\nabla\psi\right) + V\psi = E\psi$$

Applications of Schrodinger Solver

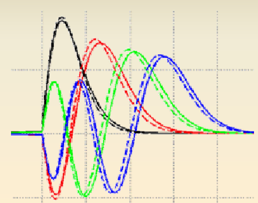


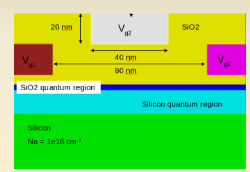


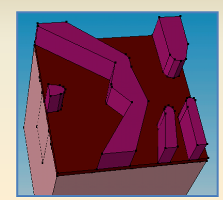


Self-Consistent Poisson-Schrodinger Solver

Applications of Self-Consistent P-S Solver







Schrodinger Solver

Time-independent Schrodinger equation:

$$\frac{-\hbar^2}{2}\nabla\left(\frac{1}{m^*}\nabla\psi(r)\right)+V(r)\psi(r)=E\psi(r)$$

Apply finite element method ⟶ Eigenvalue problem: [H] [ψ] = [E] [ψ]

⟶ Solved by Sandia high-performance eigensolver (Anasazi)

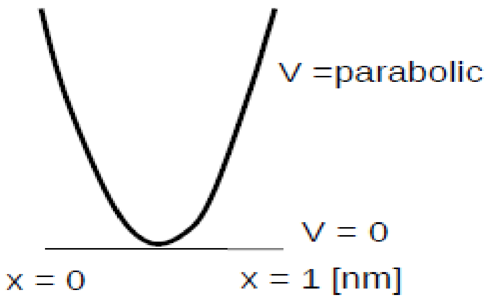
Three types of boundary conditions:

- Flux conservation b.t.w. different materials: $\frac{1}{m_1^*}\nabla\psi_1\bullet\hat{\eta}_1=\frac{1}{m_2^*}\nabla\psi_2\bullet\hat{\eta}_2$
- Neumann condition: $\frac{1}{m^*}\nabla\psi\bullet\hat{\eta}=0$
- Dirichlet condition: $\psi=0$

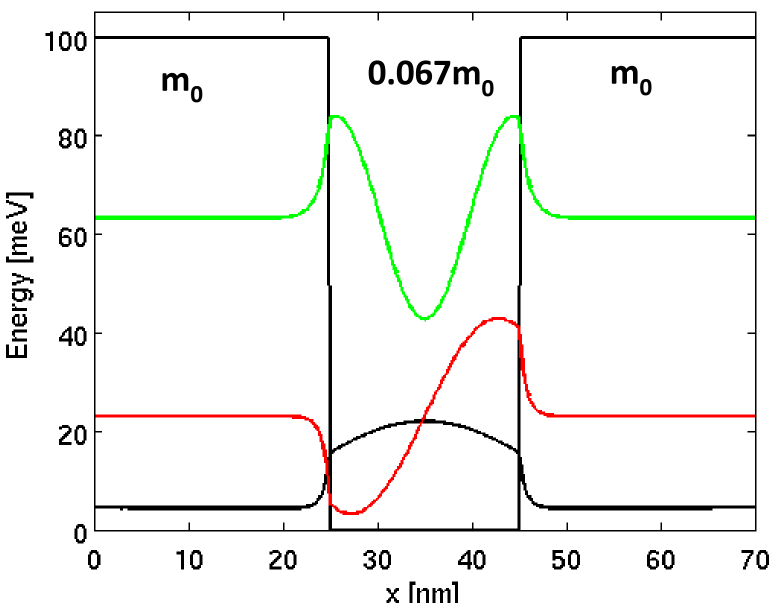
Automatically satisfied in the finite element framework

Schrodinger Solver – Application 1D

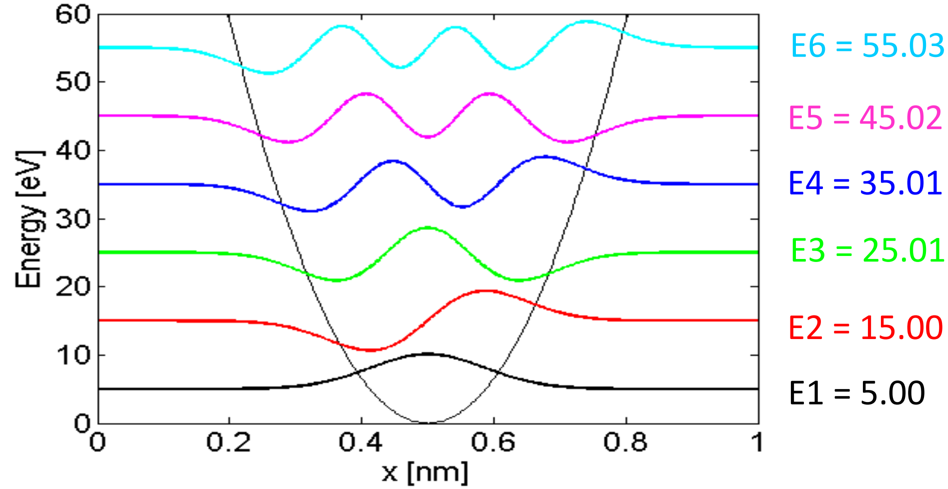
Apply the Schrodinger solver to a 1D parabolic potential well



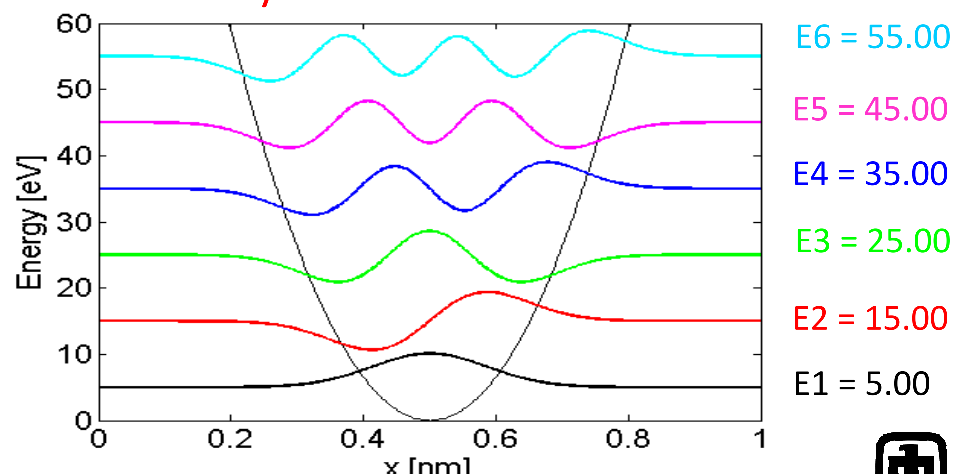
$\psi(x)$ and $\frac{1}{m^*}\frac{\partial}{\partial x}\psi(x)$ are continuous b.t.w. different materials



QCAD wave functions



Analytic wave functions



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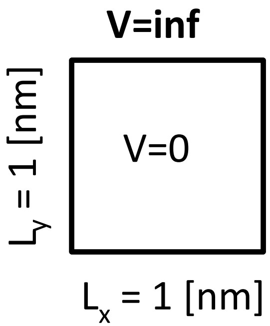
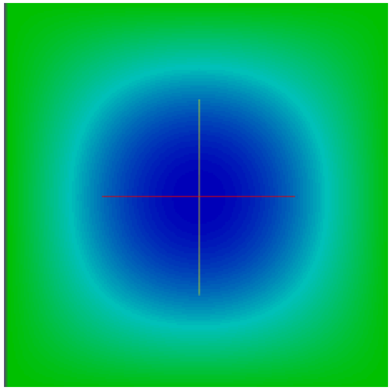
Schrodinger Solver – Application 2D

Apply the Schrodinger solver to a 2D square infinite potential well

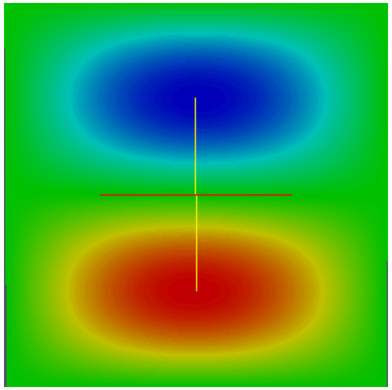


	QCAD	Analytic
E1 [eV]	0.7521	0.7521
E2 [eV]	1.8805	1.8802
E3 [eV]	1.8805	1.8802
E4 [eV]	3.0088	3.0084
E5 [eV]	3.7616	3.7605
E6 [eV]	3.7616	3.7605

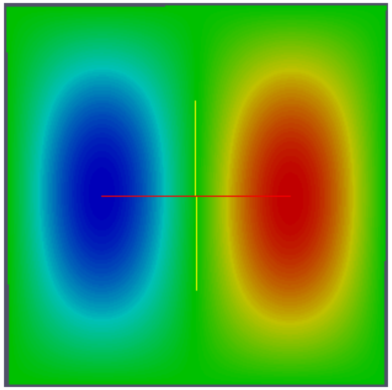
QCAD 1st WF



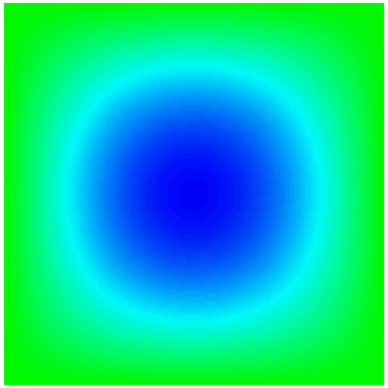
QCAD 2nd WF



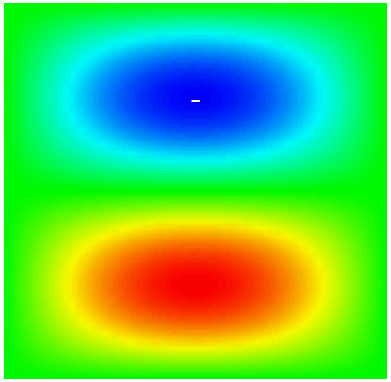
QCAD 3rd WF



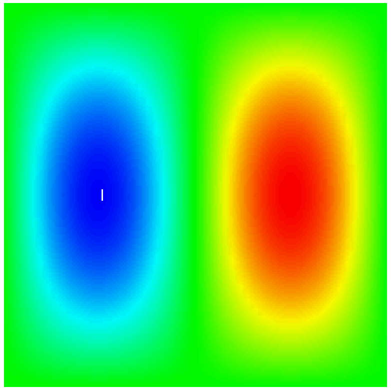
Analytic 1st WF



Analytic 2nd WF

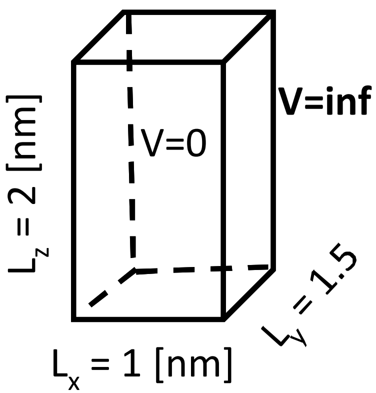


Analytic 3rd WF



Schrodinger Solver – Application 3D

Apply the Schrodinger solver to a 3D cube infinite potential well

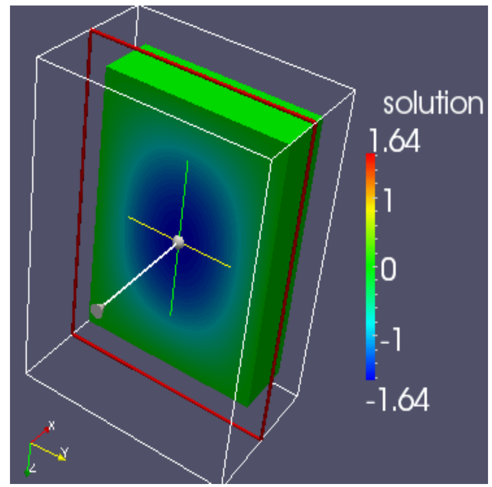


Analytic normalized WFs

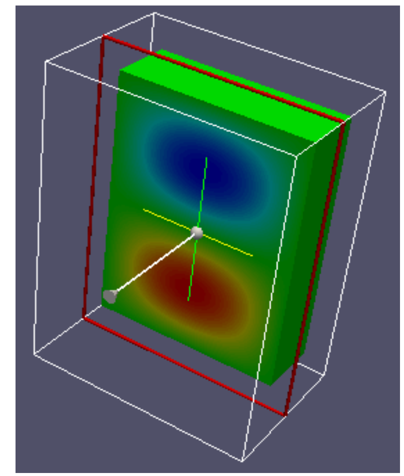
$$\psi(x,y,z)=\sqrt{\frac{8}{L_x L_y L_z}}\sin\left(\frac{\pi n_x x}{L_x}\right)\sin\left(\frac{\pi n_y y}{L_y}\right)\sin\left(\frac{\pi n_z z}{L_z}\right)$$

	QCAD	Analytic
E1 [eV]	0.6382	0.6373
E2 [eV]	0.9215	0.9194
E3 [eV]	1.1419	1.1387
E4 [eV]	1.3972	1.3895

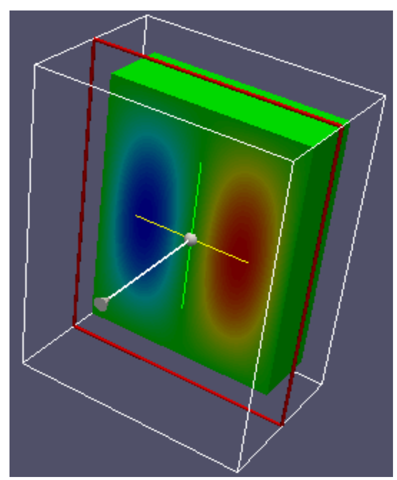
1st WF ($n_x=n_y=n_z=1$)



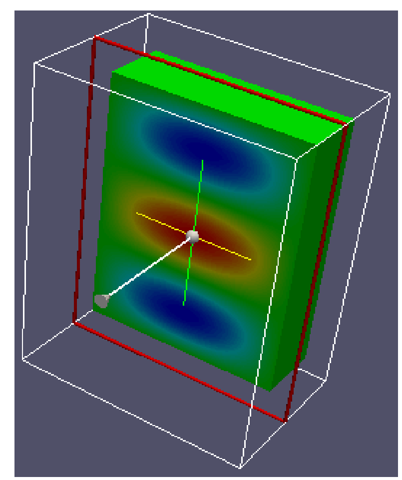
2nd WF ($n_x=n_y=1$, $n_z=2$)



3rd WF ($n_x=n_z=1$, $n_y=2$)



4th WF ($n_x=n_y=1$, $n_z=3$)



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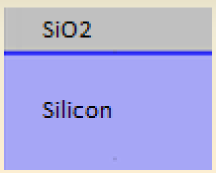
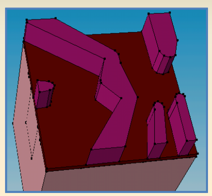
Poisson Solver Background

$$-\nabla(\varepsilon_s \nabla \phi) = q(p - n + N_D^+ - N_A^-)$$

Applications of Poisson Solver





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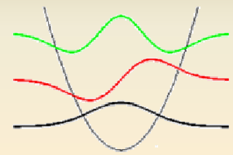
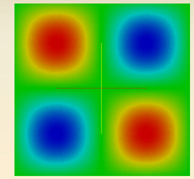
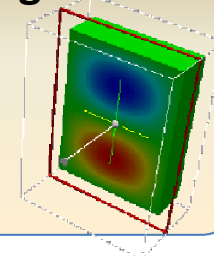
$$-\frac{\hbar^2}{2}\nabla\left(\frac{1}{m^*}\nabla\psi\right) + V\psi = E\psi$$

Applications of Schrodinger Solver

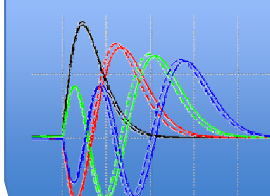


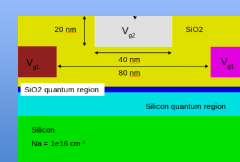


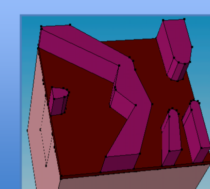


Self-Consistent Poisson-Schrodinger Solver

Applications of Self-Consistent P-S Solver







Self-Consistent Poisson-Schrodinger

Coupled Poisson equation: $-\nabla(\varepsilon_s \nabla \phi) = q[\overbrace{p(\phi) + N_D^+(\phi) - N_A^-(\phi)} - \underline{n(\phi, E_i, \psi_i)}]$

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

$N_i =$

1D (quantum well)

$$g_v \frac{m^* k_B T}{\pi \hbar^2} F_0(\eta_F)$$

2D (quantum wire)

$$g_v \left(\frac{2 m^* k_B T}{\pi \hbar^2} \right)^{1/2} F_{-1/2}(\eta_F)$$

3D (quantum dot)

$$g_v \frac{2}{1 + \exp(-\eta_F)}$$

Where $\eta_F = \dfrac{E_F - E_i}{k_B T}$ $\quad F_k(\eta_F) = \dfrac{1}{\Gamma(k+1)} \displaystyle\int_0^\infty \frac{\varepsilon^k d\varepsilon}{1 + \exp(\varepsilon - \eta_F)}$ Fermi-Dirac integral of kth order

Coupled Schrodinger equation: $\dfrac{-\hbar^2}{2} \nabla \left(\dfrac{1}{m^*} \nabla \psi_i \right) + \underline{V(\phi, n)}\psi_i = E_i \psi_i$

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

Parametrized in the Local Density Approximation [3]

[3] L. Hedin and B. I. Lundqvist, J. Phys. C **4**, 2064 (1971).

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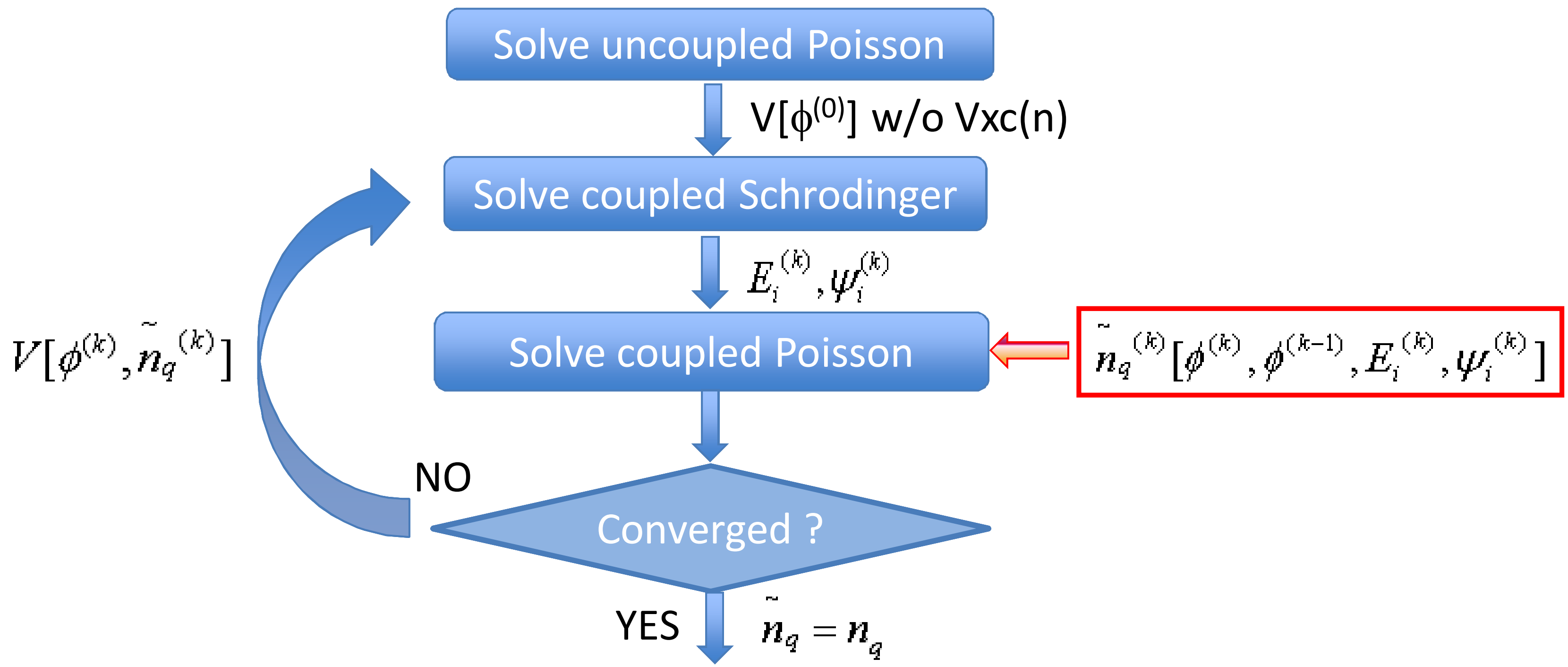
Self-Consistent Poisson-Schrodinger

Simple/Direct iteration of Poisson and Schrodinger leads to divergence due to strong coupling b.t.w. them.

Predictor-corrector iteration scheme [4] modifies quantum electron density calculation:

$n_q(E_i, \psi_i)$ with $\eta_F = \dfrac{E_F - E_i}{k_B T}$ → $\tilde{n}_q^{(k)}[\phi^{(k)}, \phi^{(k-1)}, E_i^{(k)}, \psi_i^{(k)}]$ with $\tilde{\eta}_F^{(k)} = \dfrac{E_F - E_i + q[\phi^{(k)} - \phi^{(k-1)}]}{k_B T}$



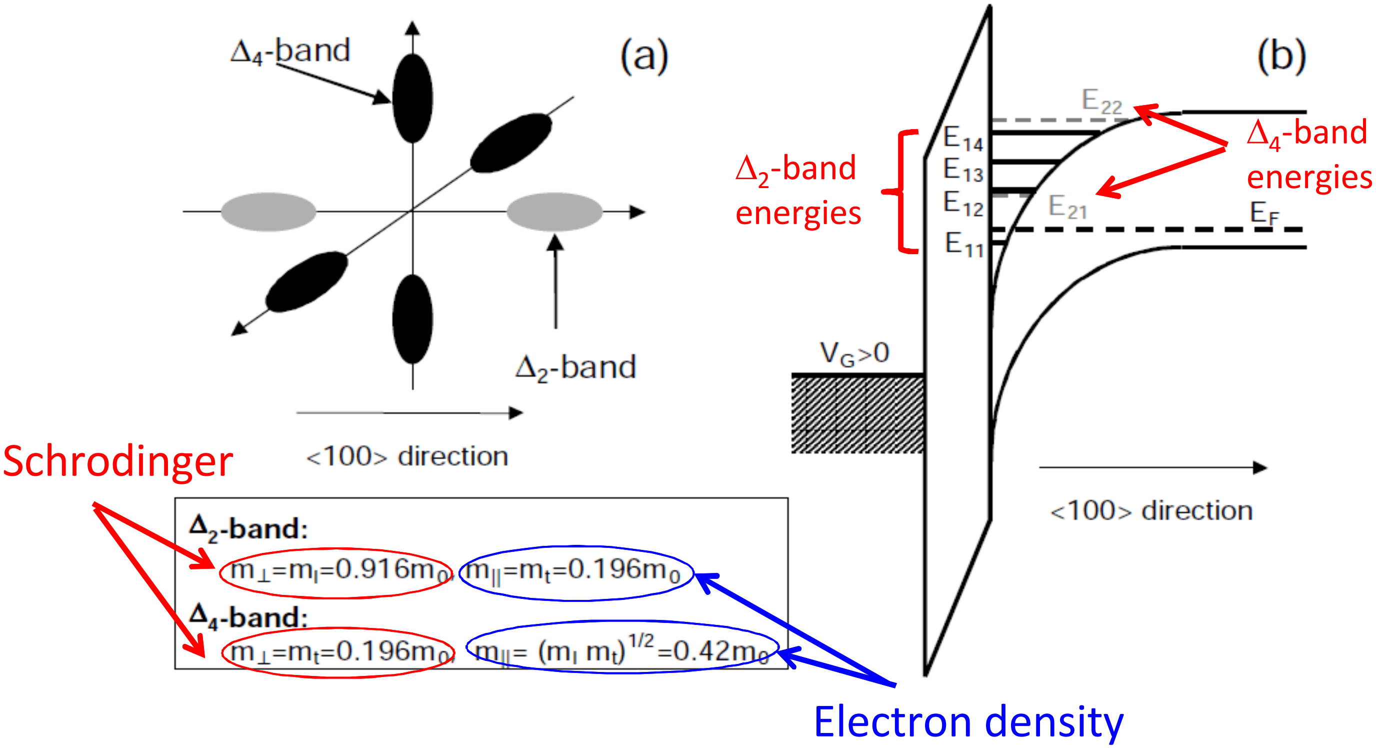
[4] A. Trellakis, A. T. Galick, A. Pacelli, and U. Ravaioli, J. Appl. Phys. **81**, 7880 (1997).

P-S Special Considerations in Silicon

Two special considerations in Silicon:

- Bulk Silicon has six equivalent conduction band minima, which degeneracy is lifted in confined Silicon.
- Effective mass tensor is anisotropic, so the effective mass in the Schrodinger equation is different from that used in calculating electron density.

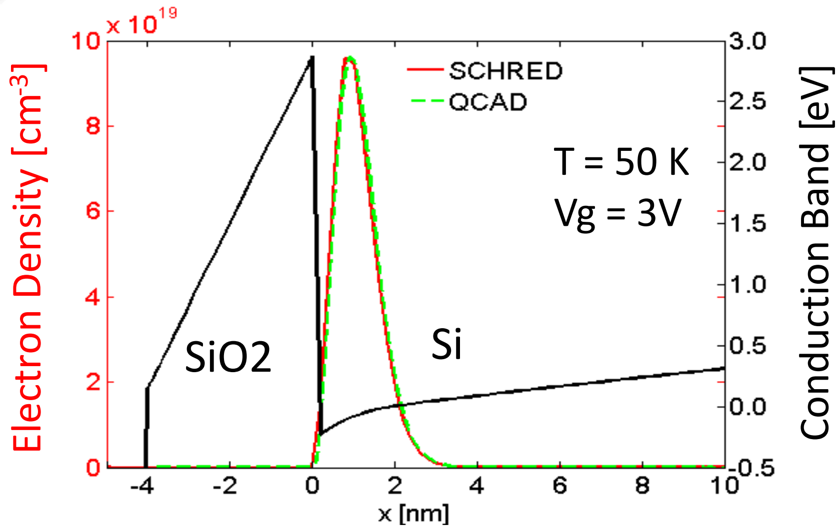
Example: 1D-confined Silicon

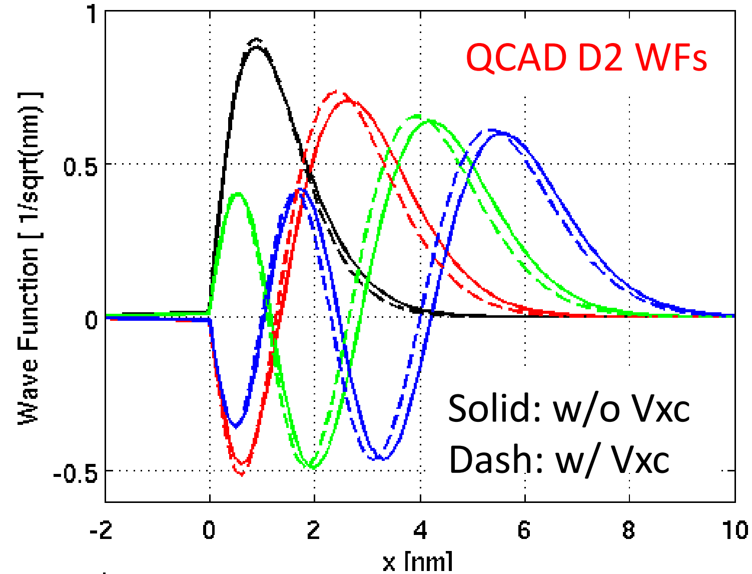


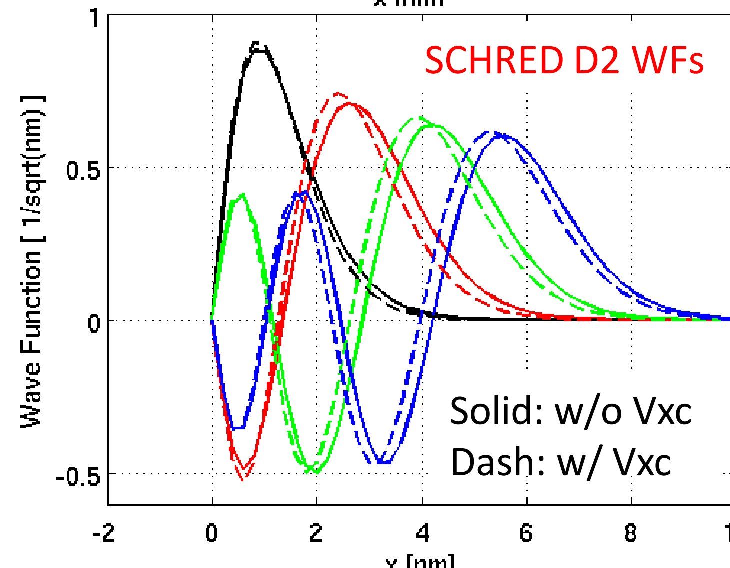
QCAD currently solves only the Δ_2-band due to its lower energy and the targeted low-T applications, while QCAD can be easily adapted to include other four valleys.

Self-Consistent P-S – Application 1D

Test structure: 1D MOS capacitor with tox = 4 nm, Na = 5e17 cm^{-3}





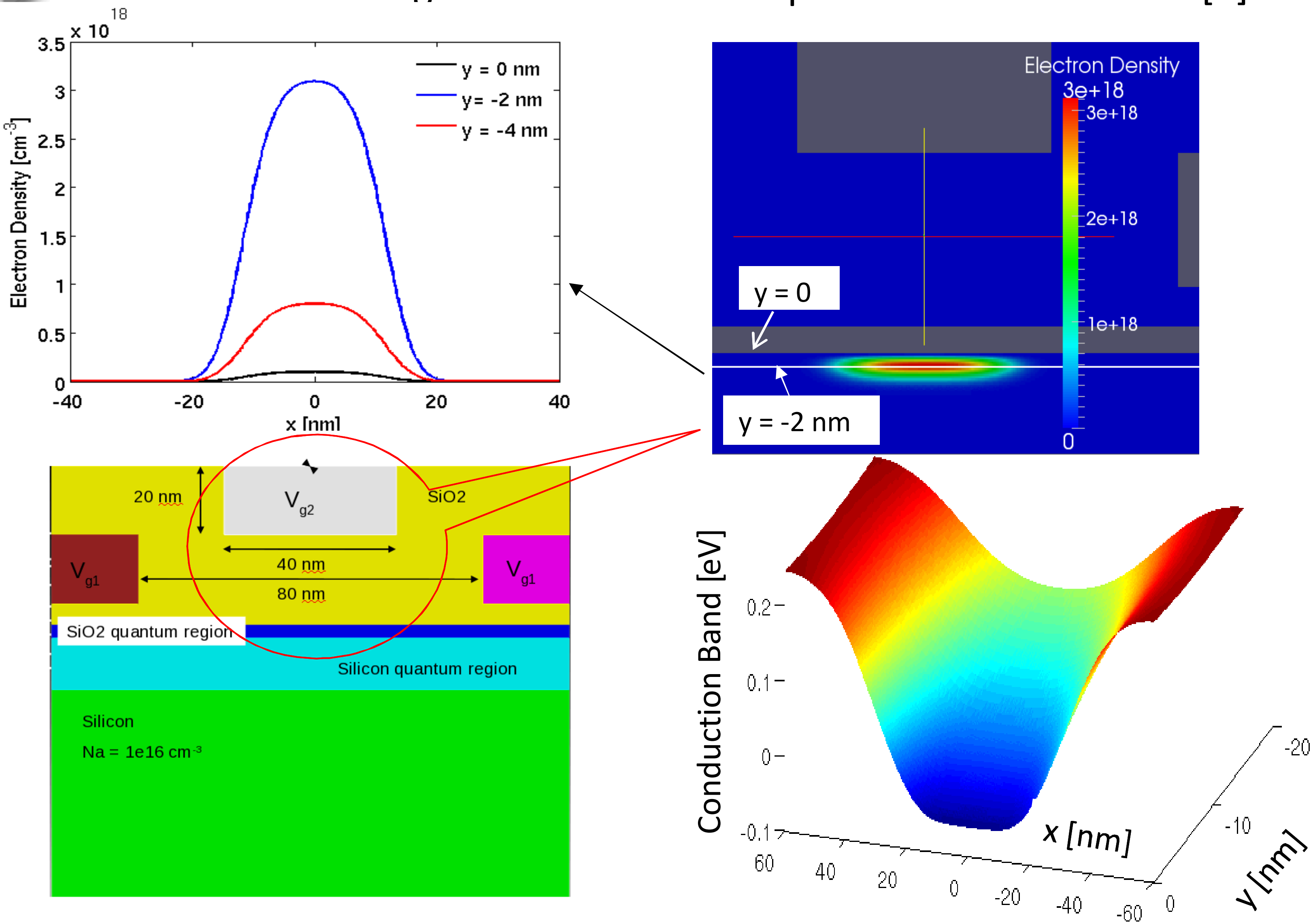


[meV]	SCHRED (w/o Vxc)	QCAD (w/o Vxc)	**SCHRED (w/ Vxc)**	**QCAD (w/ Vxc)**
E11	-71.76	-72.54	-73.68	-74.50
E12	26.12	26.71	45.63	45.72
E13	89.22	90.73	118.83	118.94
E14	142.27	144.69	175.60	176.10

With Vxc, energy separation increases and wfs become more spatial confined.

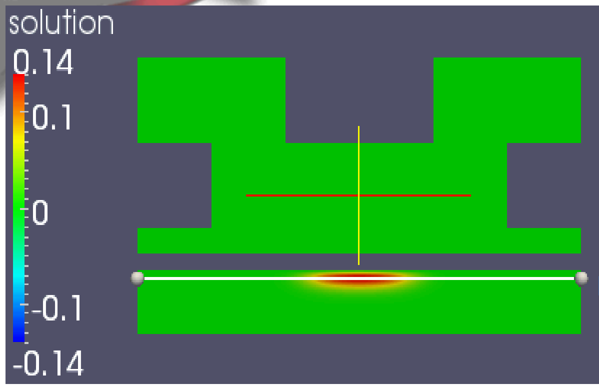
Self-Consistent P-S – Application 2D

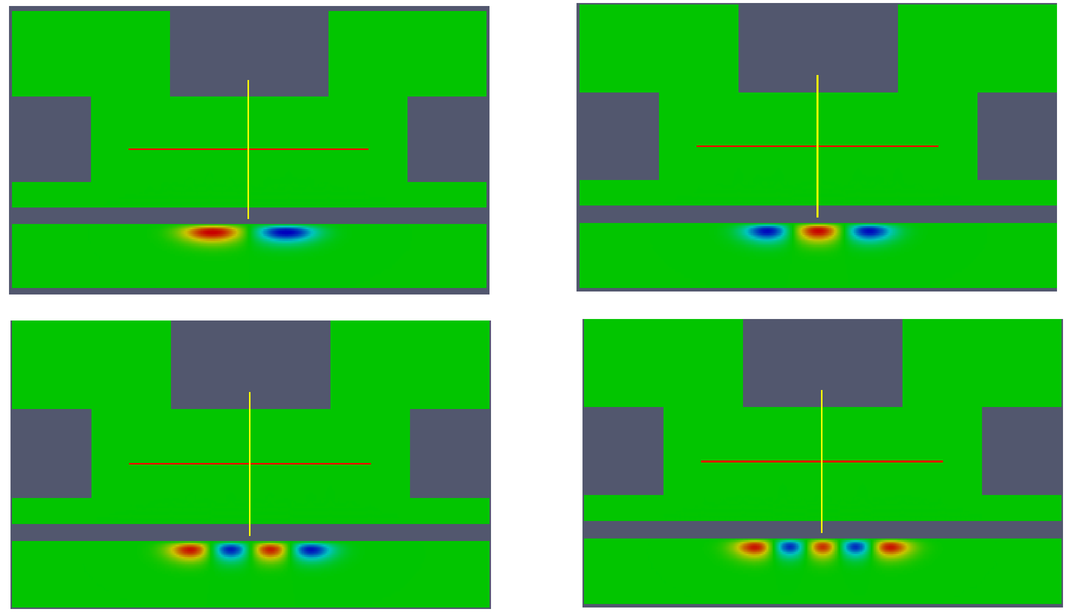
Test structure: gate-induced Silicon quantum wire from Ref. [5]



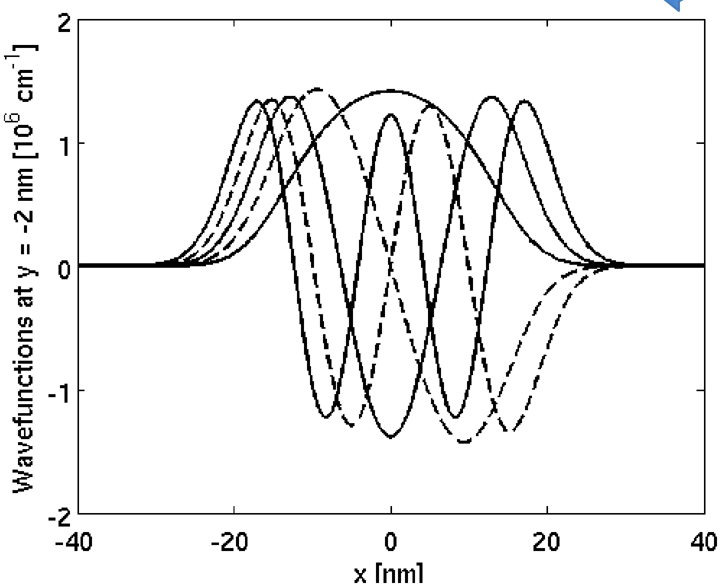
[5] Steven E. Laux and Frank Stern, Appl. Phys. Lett. **49**, 91 (1986).

Self-Consistent P-S – Application 2D





QCAD Wfs at y = -2 nm



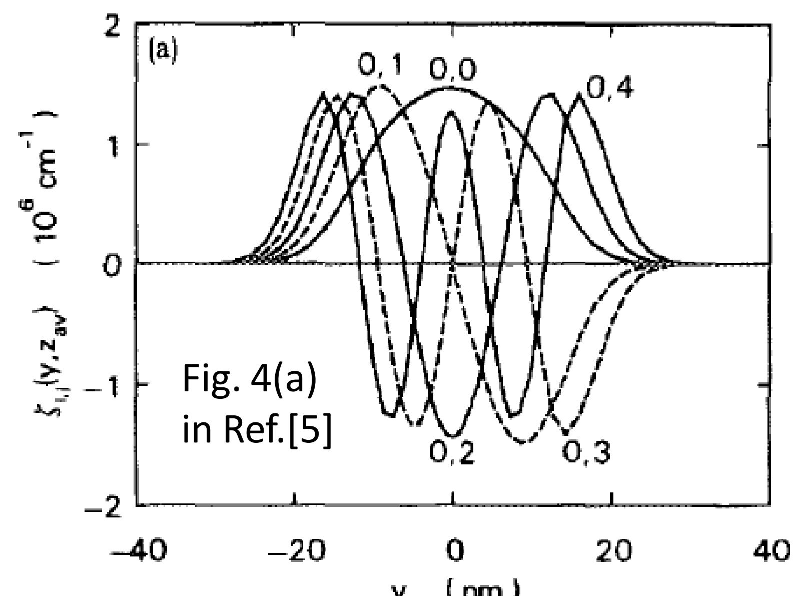


Fig. 4(a)
in Ref.[5]

Conclusion

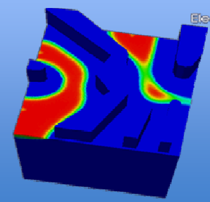
Discuss details of three QCAD solvers

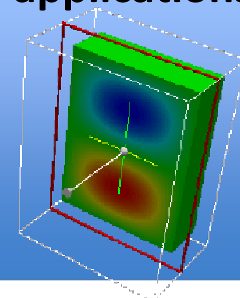
$$-\nabla(\varepsilon_s \nabla \phi) = q(p - n + N_D^+ - N_A^-)$$

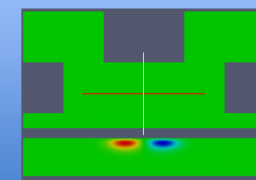
$$\frac{-\hbar^2}{2}\nabla\left(\frac{1}{m^*}\nabla\psi\right) + V\psi = E\psi$$

$$n(\phi, E_i, \psi_i) \leftrightarrow V(\phi, n)$$

Demonstrate applications of QCAD solvers







Physics-based and robust QCAD tool for quantum devices modeling

Develop new capabilities

Simulate experimental quantum dots to provide feedback and design guidance for experiment

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