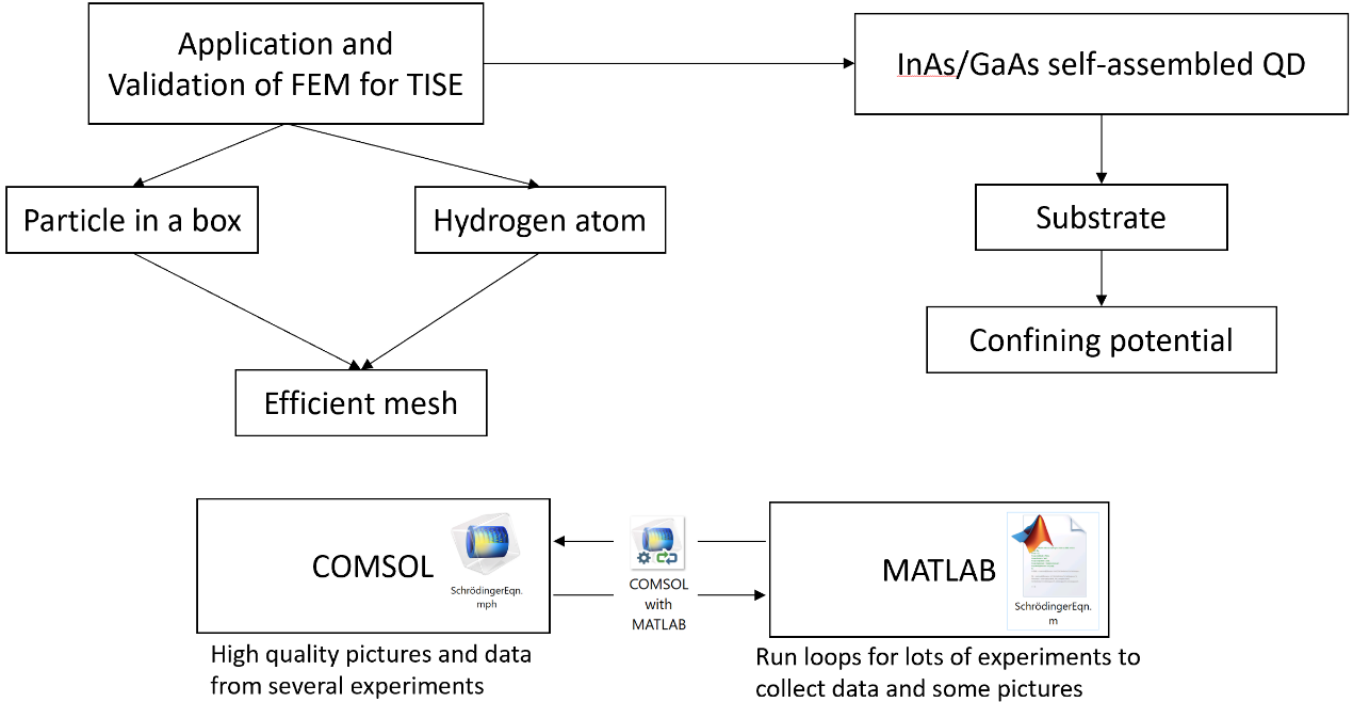
Modeling Confinement in Quantum Dot Solar Cells

Jinye Liu and M. Zubaer Hossain
Department of Mechanical Engineering, University of Delaware

- Analytical solution vs. COMSOL simulation



- **The single-particle time-independent Schrödinger equation**

$$\hat{\mathcal{H}}\psi(x,y,z) = E\psi(x,y,z)$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(x,y,z)\right]\psi(x,y,z) = E\psi(x,y,z)$$

- **In COMSOL Multiphysics**

  - Coefficient PDE form

$$\lambda^2 e_a\psi - \lambda d_a\psi + \nabla\cdot(-c\nabla\psi - \alpha\psi + \gamma) + \beta\cdot\nabla\psi + a\psi = f \qquad \text{in } \Omega$$

with $e_a = 0, d_a = 1, \alpha = 0, \gamma = 0, \beta = 0, f = 0,$ we get,

$$\nabla\cdot(-c\nabla\psi) + a\psi = \lambda\psi$$

where $c = \frac{\hbar^2}{2m_{\text{eff}}}$, $\lambda = E$, $a = V$

• Particle in a box

- **Analytical solution**
- **One-dimensional box(infinite well)**

Electron trapped, V=0 inside, V=∞ outside

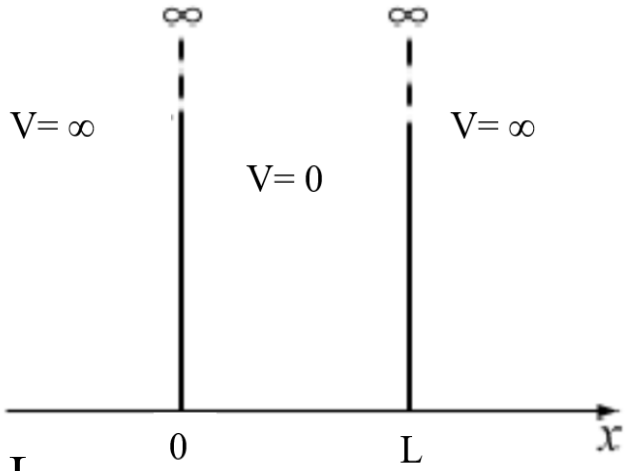
$$\left(-\frac{\hbar^2}{2m_e}\nabla^2 + 0\right)\psi(x) = E\psi(x)$$

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

ψ should be continuous ψ(x) = 0 at x = 0 and x = L

$$\psi_n(x) = A\sin\frac{n\pi x}{L} \qquad n = 1, 2, 3, 4\ldots$$

Probability of finding the particle inside the box = 1 $\int_0^L \psi^2{}_n(x)dx = 1$



$$E_n = \frac{\hbar^2\pi^2}{2m_e}\left(\frac{n^2}{L^2}\right)$$

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L}$$

• Particle in a box

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- **Three-dimensional box**

$$\left(-\frac{\hbar^2}{2m_e}\nabla^2 + 0\right)\psi_{n_x n_y n_z}(x,y,z) = E_{n_x n_y n_z}\psi_{n_x n_y n_z}(x,y,z)$$

Similar to the case of one-dimensional

$$E_{n_x n_y n_z} = \frac{\hbar^2\pi^2}{2m_e}\left[\left(\frac{n_x}{L_x}\right)^2 + \left(\frac{n_y}{L_y}\right)^2 + \left(\frac{n_z}{L_z}\right)^2\right]$$

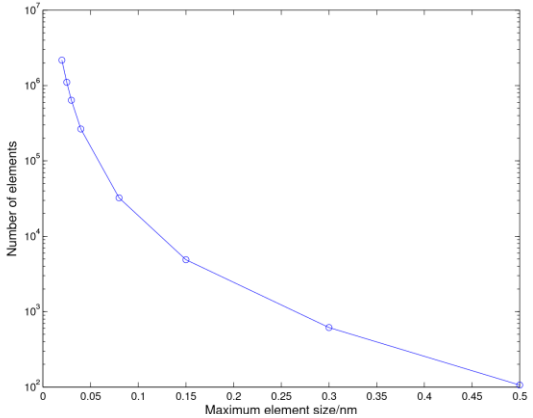
Lx=Ly=Lz=L

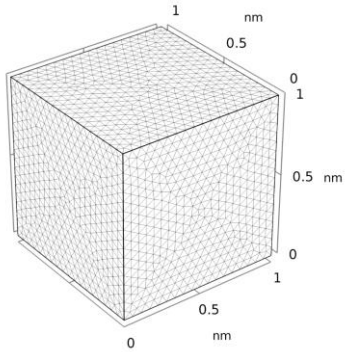
$$\psi_{n_x n_y n_z}(x,y,z) = \left(\frac{2}{L}\right)^{\frac{3}{2}} \sin\frac{n_x\pi x}{L}\sin\frac{n_y\pi y}{L}\sin\frac{n_z\pi z}{L}$$

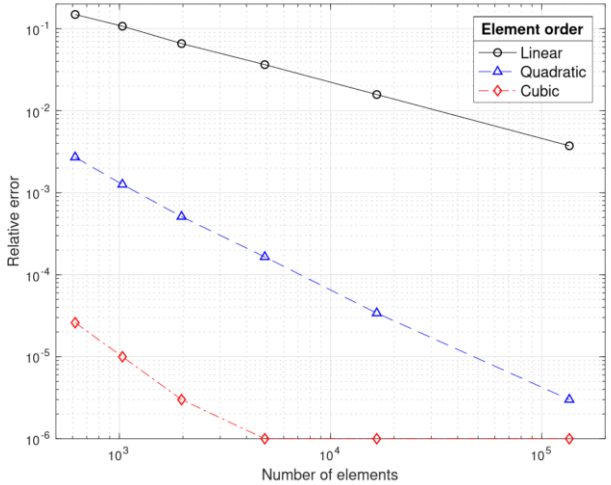
$$n_x = 1,2,3,4\ldots; n_y = 1,2,3,4\ldots; n_z = 1,2,3,4\ldots$$

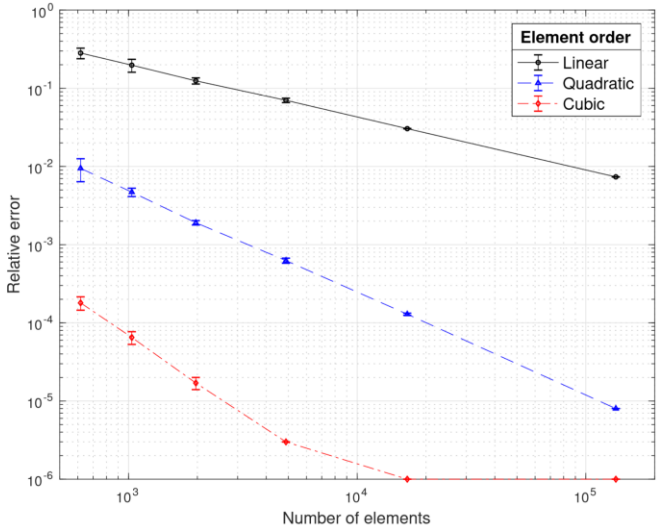
COMSOL simulation

- Element (domain) type for 3D: tets,prisms…
- Element order: linear,quadratic,cubic…
- Element size parameters: $e_{\max}, e_{\min}, e_{\mathrm{mgr}}, e_{\mathrm{cf}}\ e_{\mathrm{ronr}}$
- Optimization levels, Adaptive mesh refinement, elements' quality









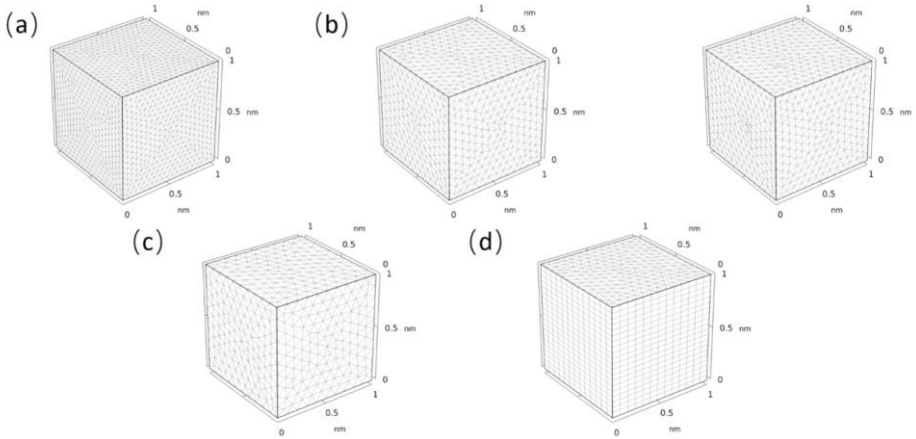
Cubic elements is better than quadratic elements

Mesh convergence study for an electron in a 3D box for ground state and first excited state

• Particle in a box

1. Mesh1: Lagrange quadratic element, predefined "finer" mesh($e_{max} = 0.055; e_{min} = 0.004; e_{mgr} = 1.4; e_{cf} = 0.4; e_{ronr} = 0.7$), Optimization Level=High

2. Mesh2: Lagrange quadratic element, predefined "fine" mesh($e_{max} = 0.055; e_{min} = 0.004; e_{mgr} = 1.4; e_{cf} = 0.4; e_{ronr} = 0.7$), Optimization Level=High, with one defaulted adaptive mesh



3. Mesh3: Lagrange cubic element, predefined "normal" mesh($e_{max} = 0.055; e_{min} = 0.004; e_{mgr} = 1.4; e_{cf} = 0.4; e_{ronr} = 0.7$), Optimization Level=High

4. Mesh4: Lagrange cubic element, predefined "fine" mesh on top($e_{max} = 0.08; e_{min} = 0.01; e_{mgr} = 1.45; e_{cf} = 0.5; e_{ronr} = 0.6$), swept mesh distribution: the number of layers is 20, Optimization Level=High

Mesh methods	DOF(domain elements)	ST	Relative error level
Mesh1	138354(100149)	82s	10^{-6} to 10^{-4}
Mesh2	99183(32324)	513s	10^{-6} to 10^{-4}
Mesh3	77740(16485)	40s	0 to 10^{-5}
Mesh4	115168(8040)	85s	0 to 10^{-5}

Mesh3,Mesh4 are more efficient and accurate. Mesh4 gives high quality elements

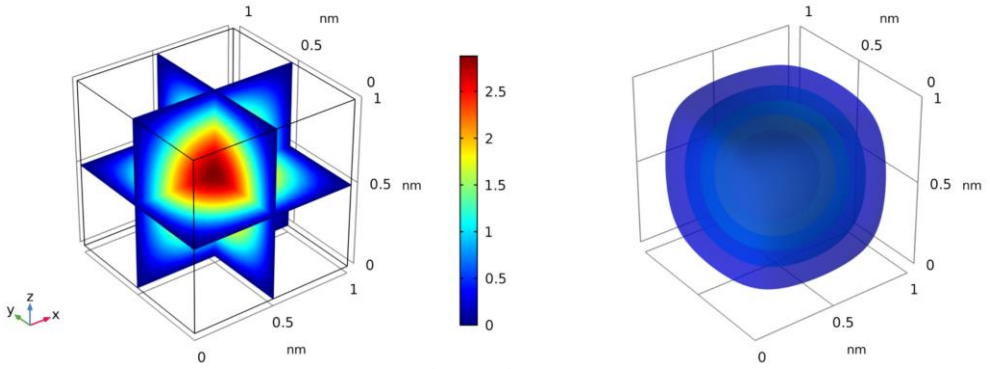
• Particle in a box

Comparison of Relative errors E_r of four mesh methods with respect to 14 distinct energy levels, all units of Relative errors are $10^{-5}[eV]$

(n_x, n_y, n_z)	$Deg.$	E_{exact}	$E_{r\ \text{mesh1}}$	$E_{r\ \text{mesh2}}$	$E_{r\ \text{mesh3}}$	$E_{r\ \text{mesh4}}$
(1,1,1)	1	1.128090	0.266	0.800	0	0
(2,1,1),(1,2,1),(1,1,2)	3	2.256180	1.06	3.06	0.0443	0
(2,2,1),(2,1,2),(1,2,2)	3	3.384270	2.33	7.12	0.0886	0.0590
(3,1,1),(1,3,1),(1,1,3)	3	4.136331	3.36	9.11	0.121	0.0484
(2,2,2)	1	4.512361	4.17	13.4	0.177	0.199
(3,2,1),(3,1,2),(2,1,3),(2,3,1),(1,2,3),(1,3,2)	6	5.264421	5.57	16.3	0.285	0.152
(3,2,2),(2,3,2),(2,2,3)	3	6.392511	8.35	26.2	0.532	0.125
(4,1,1),(1,4,1),(1,1,4)	3	6.768541	8.89	22.1	0.576	0.369
(3,1,3),(3,3,1),(1,3,3)	3	7.144571	10.2	29.1	0.728	0.391
(4,2,1),(4,1,2),(1,4,2),(2,4,1),(1,2,4),(2,1,4)	6	7.896631	12.3	34.5	0.975	0.557
(3,3,2),(2,3,3),(3,2,3)	3	8.272661	14.0	43.5	1.16	0.338
(4,2,2),(2,4,2),(2,2,4)	3	9.024721	16.2	50.0	1.46	0.488
(4,3,1),(4,1,3),(3,1,4),(3,4,1),(1,3,4),(1,4,3)	6	9.776781	19.1	53.1	1.87	1.07
(5,1,1),(1,5,1),(1,1,5),(3,3,3)	4	10.15281	2.10	6.55	0.214	0.128

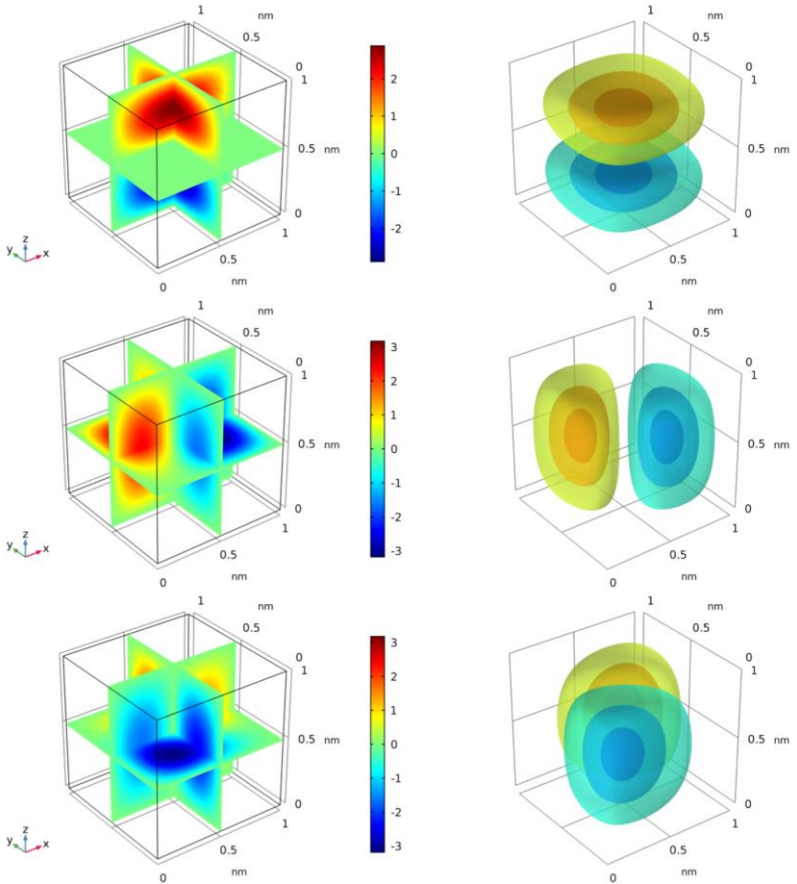
Mesh4:Accurate and efficient

• Particle in a box



(1,1,1)

Ground state electron wavefunction for an electron in a 3D box

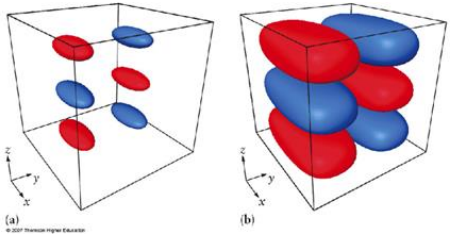


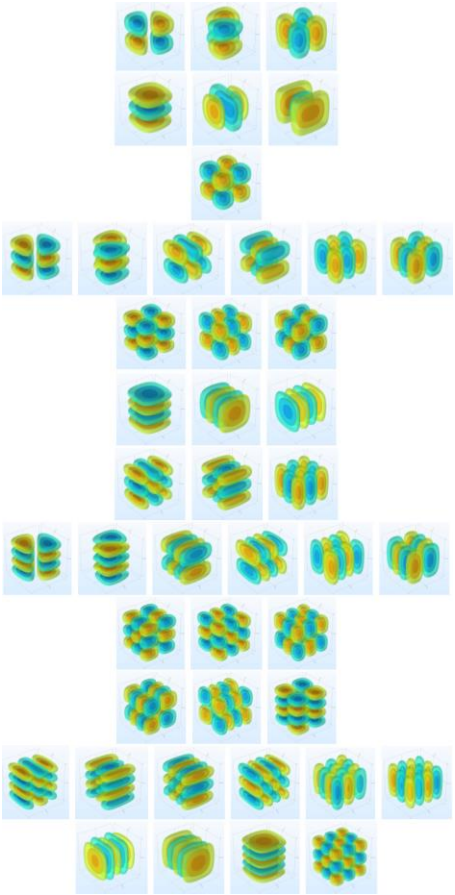
(2,1,1),(1,2,1),(1,1,2)

First excited electron wavefunction for an electron in a 3D box

• Particle in a box

n=3 to n=10 electron wave functions for an electron in a 3D box





(2,2,1),(2,1,2),(1,2,2)
(3,1,1),(1,3,1),(1,1,3)
(2,2,2)
(3,2,1),(3,1,2),(2,1,3),(2,3,1),(1,2,3),(1,3,2)
(3,2,2),(2,3,2),(2,2,3)
(4,1,1),(1,4,1),(1,1,4)
(3,1,3),(3,3,1),(1,3,3)
(4,2,1),(4,1,2),(1,4,2),(2,4,1),(1,2,4),(2,1,4)
(3,3,2),(2,3,3),(3,2,3)
(4,2,2),(2,4,2),(2,2,4)
(4,3,1),(4,1,3),(3,1,4),(3,4,1),(1,3,4),(1,4,3)
(5,1,1),(1,5,1),(1,1,5),(3,3,3)

• Hydrogen atom

• Analytical solution

$$V_{\text{atom}} = -\frac{e^2}{4\pi\epsilon_0\sqrt{x^2+y^2+z^2}}$$

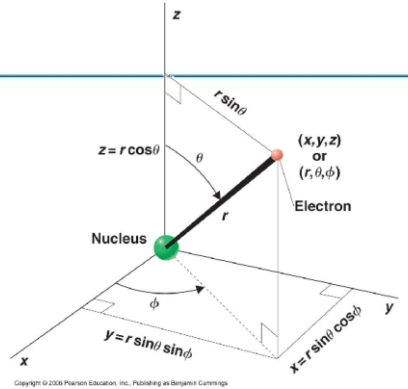
$$\left(-\frac{\hbar^2}{2m_e}\nabla^2 + V\right)\psi(x,y,z) = E\psi(x,y,z)$$

$$\psi(x,y,z) \rightarrow \psi(r,\theta,\varphi)$$

$$x = r\sin\theta\cos\varphi$$
$$y = r\sin\theta\sin\varphi$$
$$z = r\cos\theta$$

$$\frac{1}{r^2}\left(\frac{\partial}{\partial r}r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2}$$

$$+\frac{2m}{\hbar^2}\left(E + \frac{e^2}{4\pi\varepsilon_0 r}\right)\psi = 0$$



$$E_n = -\frac{1}{n^2}\frac{m_e e^4}{8\epsilon_o^2 h^2}$$

$$\psi(r,\theta,\varphi) = R_{n,l}(r)Y_{l,m_l}(\theta,\varphi)$$

$$\psi_{100}(r,\theta,\varphi) = R_{10}(r)Y_{00}(\theta,\varphi) = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2} e^{-\frac{r}{1a_0}}$$

$$\psi_{200}(r,\theta,\varphi) = R_{20}(r)Y_{00}(\theta,\varphi) = \frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_0}\right)^{3/2}\left(2 - \frac{r}{a_0}\right)e^{-\frac{r}{2a_0}}$$

$$\text{n} = 1,2,3\ldots \quad l = 0,1,2\ldots(n-1),\ m_l = 0,\pm1,\pm2,\ldots,\pm l$$

• Hydrogen atom

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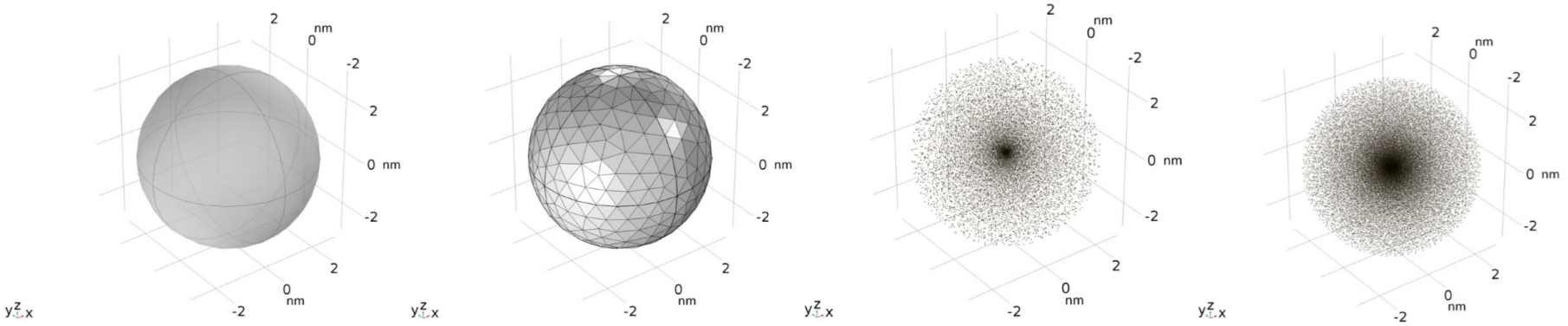
- **Analytical solution**

a_o=0.5292Å,e=1.6022e-19[C],m_e=9.1094e-31[kg],ϵ_o=8.8542e-12[F/m],h=6.6261e-34[J· s]				
(n,l,m)	R_{nl}	$Y_l^{m_l}$	ψ_{nlm_l}	$E_{n_{\text{exact}}}$
$(1,0,0)$	$2\left(\frac{1}{a_o}\right)^{\frac{3}{2}} e^{-\frac{r}{a_o}}$	$\frac{1}{\sqrt{4\pi}}$	$\frac{1}{\sqrt{\pi}}\left(\frac{1}{a_o}\right)^{\frac{3}{2}} e^{-\frac{r}{a_o}}$	-13.6062
$(2,0,0)$	$\frac{1}{2\sqrt{2}}\left(\frac{1}{a_o}\right)^{\frac{3}{2}}\left(2-\frac{r}{a_o}\right) e^{-\frac{r}{2a_o}}$	$\frac{1}{\sqrt{4\pi}}$	$\frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_o}\right)^{\frac{3}{2}}\left(2-\frac{r}{a_o}\right) e^{-\frac{r}{2a_o}}$	-3.4015
$(2,1,0)$	$\frac{1}{2\sqrt{6}}\left(\frac{1}{a_o}\right)^{\frac{3}{2}}\left(\frac{r}{a_o}\right) e^{-\frac{r}{2a_o}}$	$\frac{\sqrt{3}}{2\sqrt{\pi}} cos(\theta)$	$\frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_o}\right)^{\frac{3}{2}}\left(\frac{r}{a_o}\right) e^{-\frac{r}{2a_o}} cos(\theta)$	-3.4015
$(2,1,\pm1)$	$\frac{1}{2\sqrt{6}}\left(\frac{1}{a_o}\right)^{\frac{3}{2}}\left(\frac{r}{a_o}\right) e^{-\frac{r}{2a_o}}$	$\frac{\sqrt{3}}{2\sqrt{2\pi}} sin(\theta) e^{\pm i\phi}$	$\frac{1}{8\sqrt{\pi}}\left(\frac{1}{a_o}\right)^{\frac{3}{2}}\left(2-\frac{r}{a_o}\right) e^{-\frac{r}{2a_o}} sin(\theta) e^{\pm i\phi}$	-3.4015

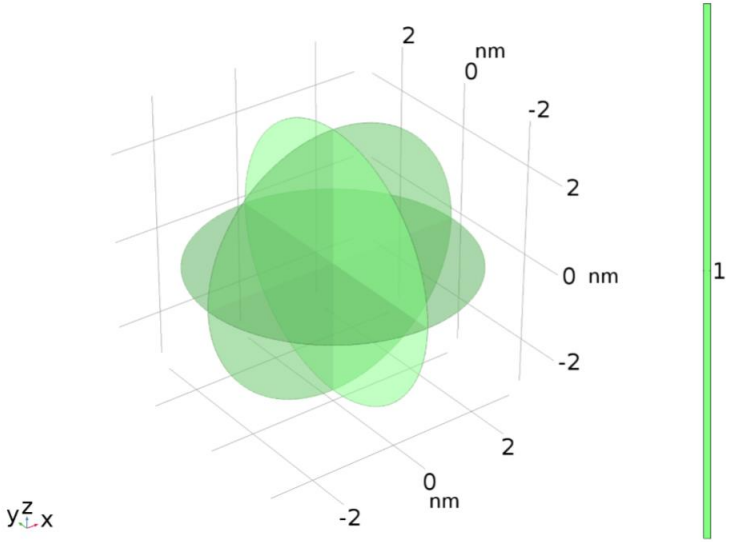
• Hydrogen atom

• COMSOL simulation



- Shrink elements with a scale factor 0.05
- No. of quadratic elements is much greater than No. of cubic elements
- Denser mesh for the core of hydrogen atom where the electron wave functions are localized

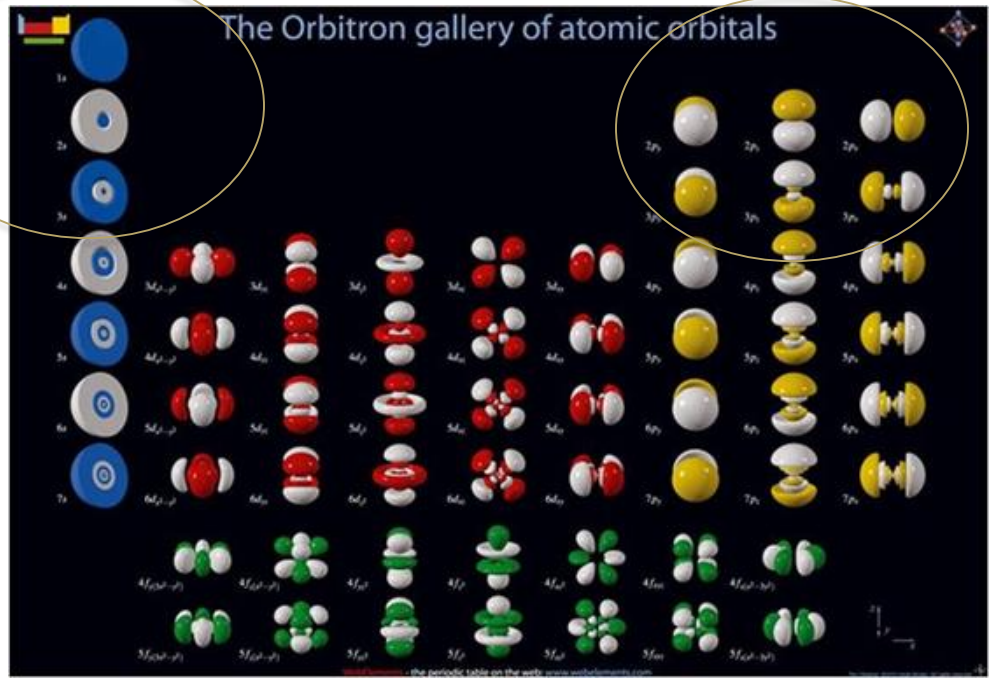
• Hydrogen atom



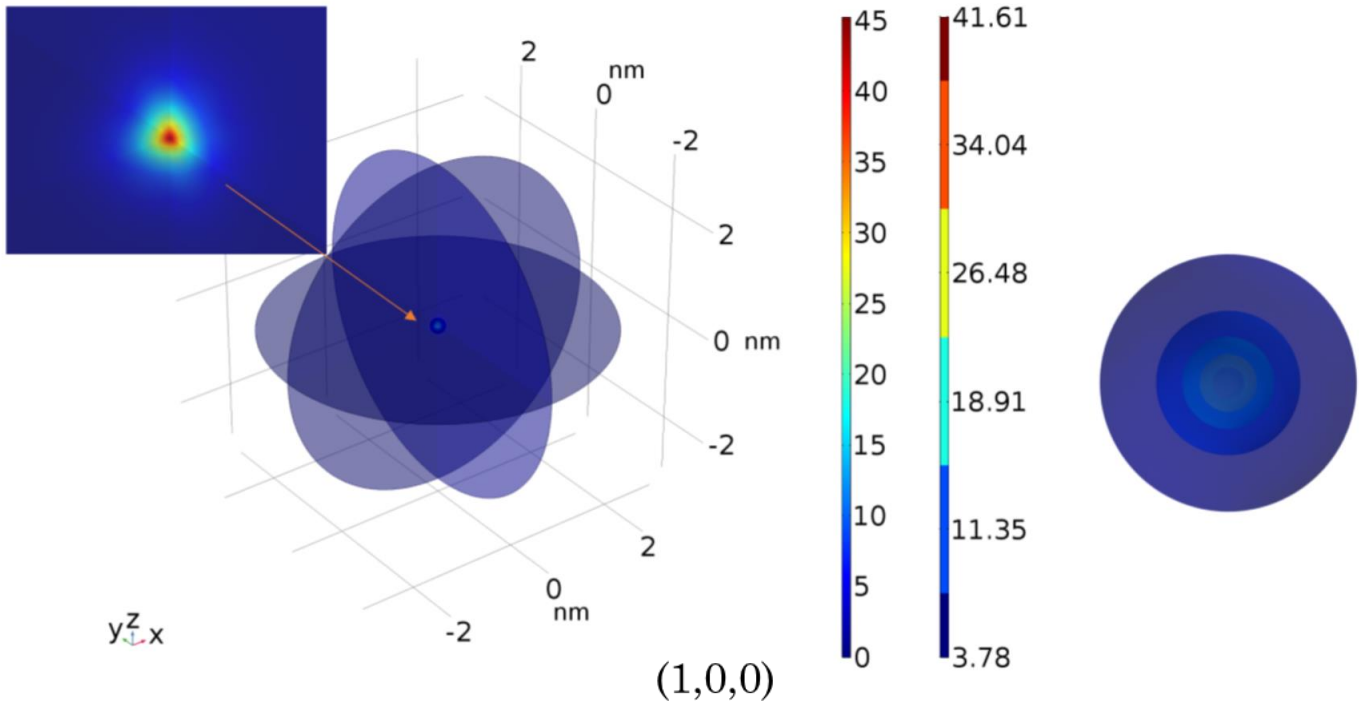
Normalization of wave functions for the hydrogen atom, the figure shows the integral of $u2$ modulus square for the entire domain equals 1. there are no propability for an electron to go outside of this domain

• Hydrogen atom

- **Compared with two existing hydrogen electron orbitals**

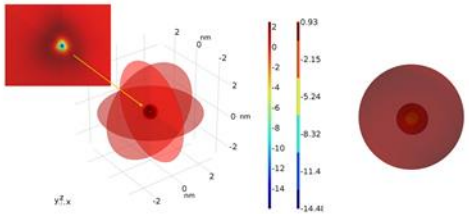


• Hydrogen atom

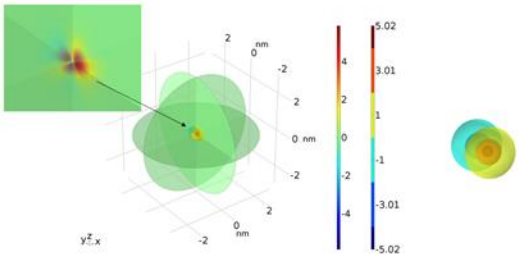


Ground state electron wavefunction of the hydrogen atom, quantum number:(n, l, m)=(1,0,0), there is one 1s orbital

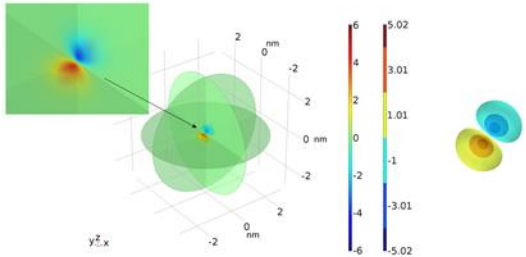
• Hydrogen atom



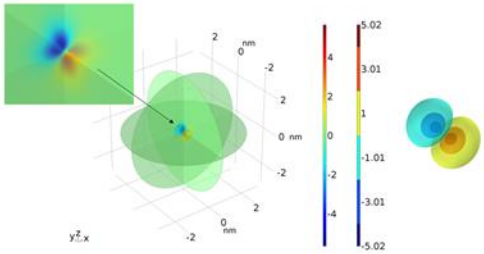
(2,0,0)



(2,1,-1)



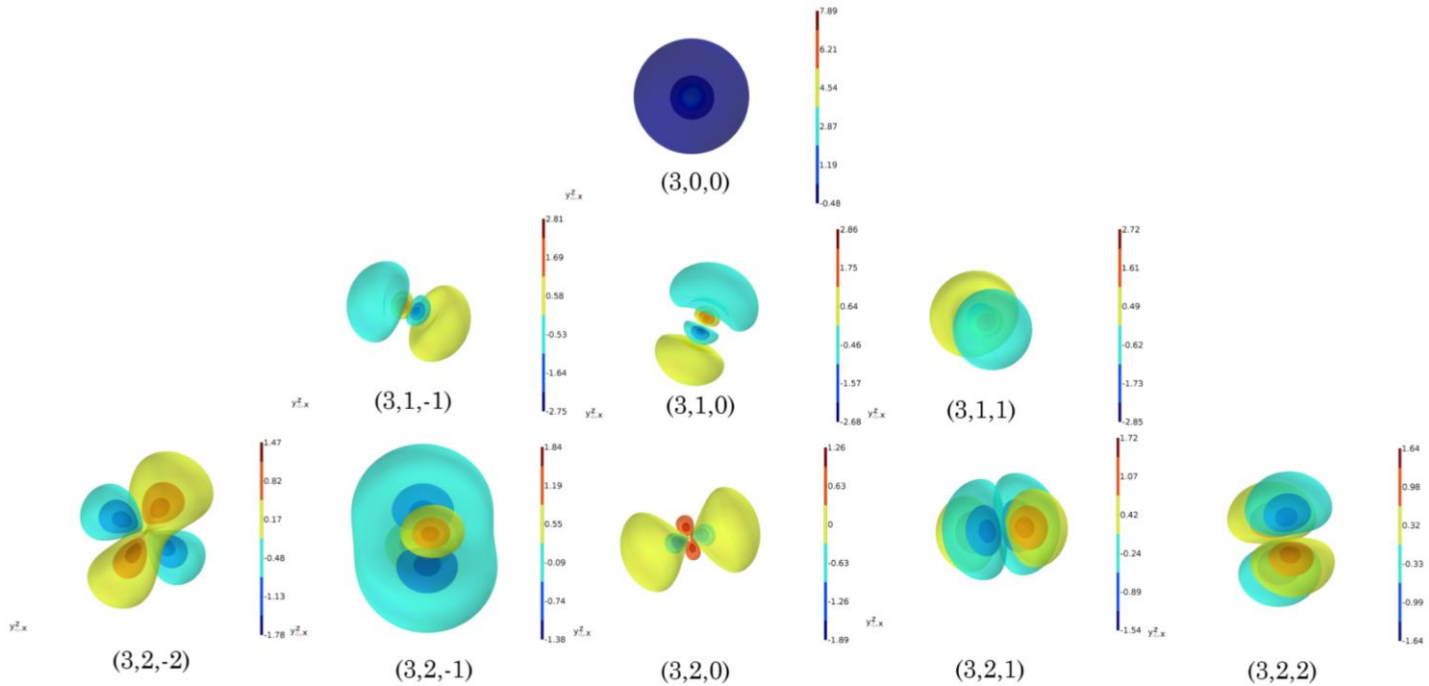
(2,1,0)



(2,1,1)

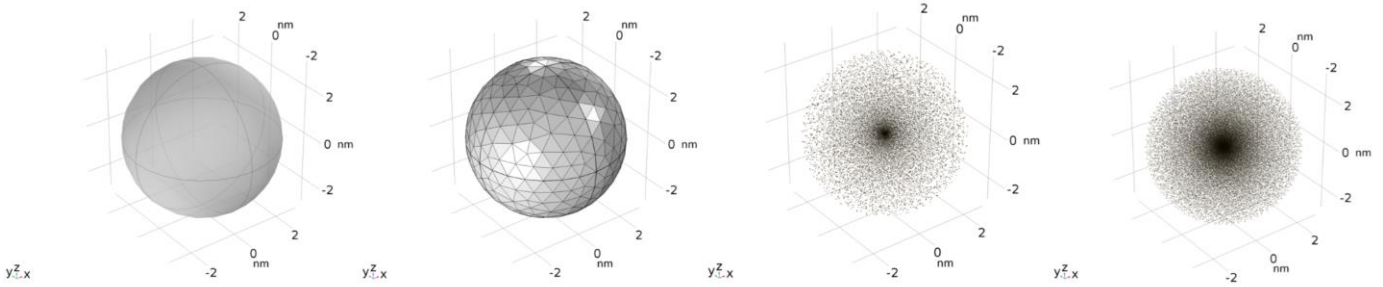
First excited state electron wavefunction of the hydrogen atom, quantum number:(n, l, m)=(2,0,0),(2,1,-1),(2,1,0),(2,1,1), there are one 2s orbital and three 2p orbitals

• Hydrogen atom



By using isosurface function with 6 levels in COMSOL, we can get the shape of wave functions as well as the associated values of these 6 levels. First excited state electron wavefunction of the hydrogen atom, quantum number:(n,l,m)=(2,0,0),(2,1,-1),(2,1,0),(2,1,1), there are one 3s orbital, three 3p orbitals and five 3d orbitals

• Hydrogen atom

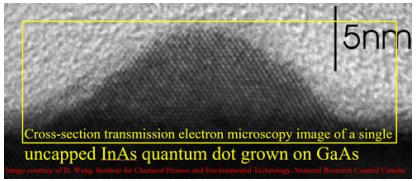


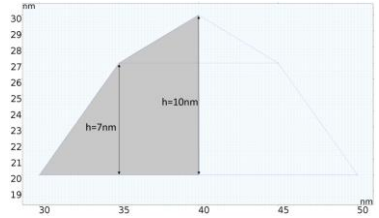
element orders	mesh expression	No.	DOF	$E_{(1,0,0)}$	$E_{(2,0,0)}$	$E_{(2,1,0)}$	$E_{(2,1,1)}$	$E_{(2,1,-1)}$
quadratic	$0.154 * sqrt(x^2 + y^2 + z^2) + 0.01$	106725	143684	-13.5805	-3.3980	-3.4011	-3.4011	-3.4011
cubic	$0.24 * sqrt(x^2 + y^2 + z^2) + 0.01$	31561	143540	-13.6077	-3.4017	-3.4015	-3.4015	-3.4015

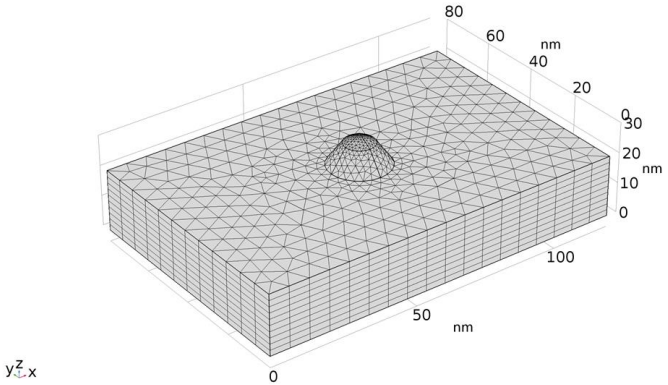
Cubic elements are better

Self-assembled quantum dot

$$\nabla \cdot (-c\nabla\psi) + a\psi = \lambda\psi \quad \text{where } c = \frac{\hbar^2}{2m_{\text{eff}}},\ \lambda = E\,,\ a = V$$



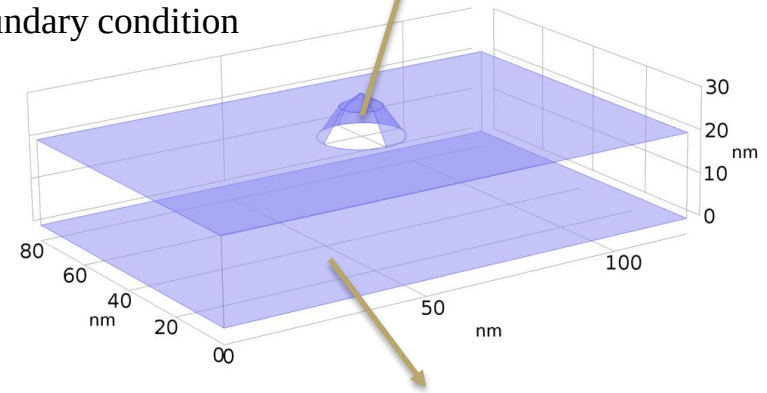




$$m_{\text{InAs}} = 0.023m_{\text{e}}$$

Vqd=0

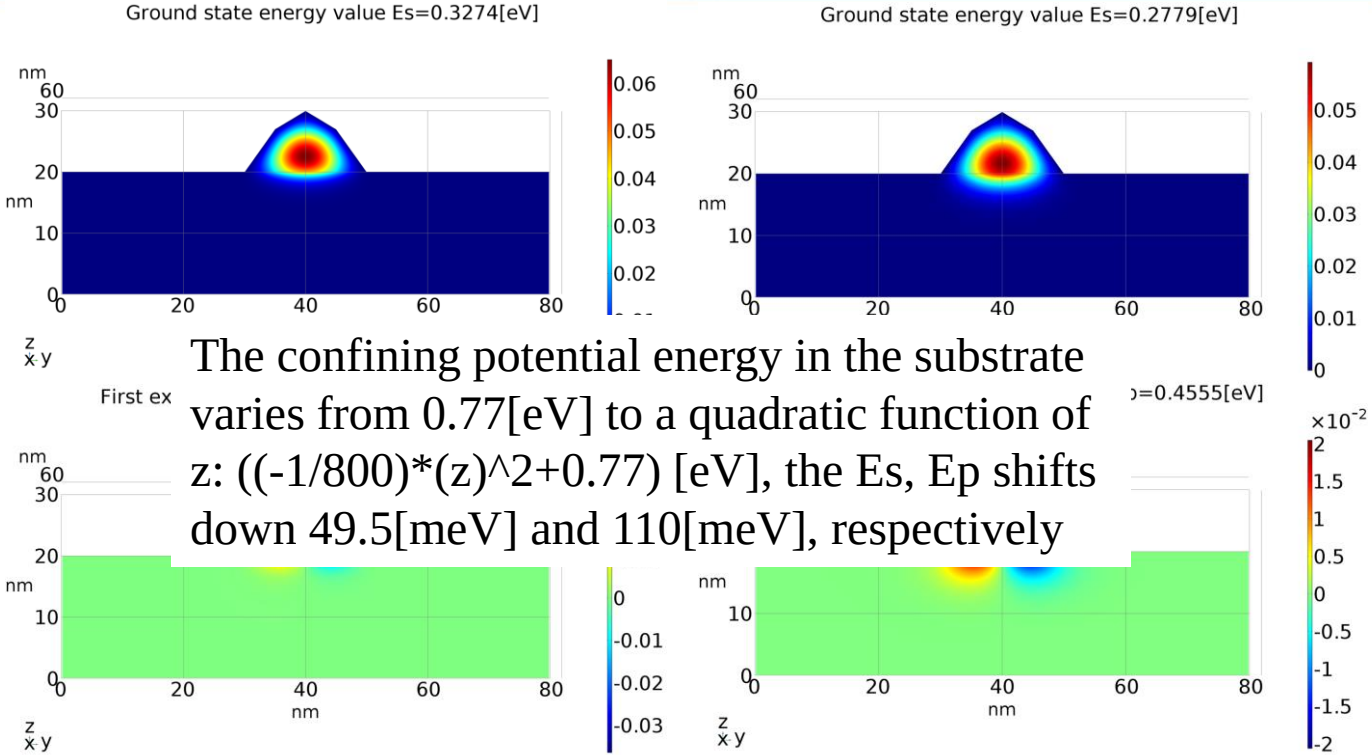
Dirichlet boundary condition



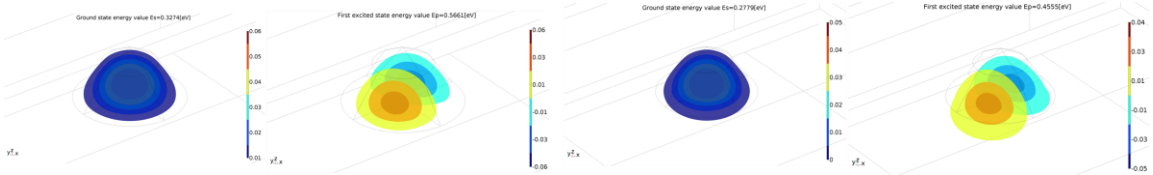
$$m_{\text{GaAs}} = 0.067m_{\text{e}}$$

$$V_{\text{substrate1}} = 0.77$$

$$V_{\text{substrate2}} = V(z) = ((-1/800) * z^2 + 0.77) \qquad z \in [0, 20]$$



The confining potential energy in the substrate varies from 0.77[eV] to a quadratic function of z: ((-1/800)*(z)^2+0.77) [eV], the Es, Ep shifts down 49.5[meV] and 110[meV], respectively



Conclusion

- Mesh convergence study(different order elements, particle in a box problem)
- Validate “particle in a box” and “hydrogen atom” problems by comparing with its analytical solutions and 3D models.
- Efficient mesh method (mesh the domains where the electron localized with cubic, high quality elements)
- The confining potential of the substrate plays an important role in engineering electron energies as well as wave functions in QDs

Thank you for your listening !

Questions?