Modeling Confinement in Quantum Dot Solar Cells

J. Liu and M. Zubaer Hossain

Department of Mechanical Engineering, University of Delaware, Newark, DE 19716, USA

INTRODUCTION: For the fact that each bandgap of single solar cell is fixed, it is advancing a technology called quantum dot solar cell (QDSC) that could manipulate quantized energy levels to absorb sunlight by varying quantum dot's parameters. In addition to exploring the effect of size and shape of QD[2] on confinement, it is of great significance to understand the mechanistic coupling between a quantum dot and the substrate on which it is grown. The schemes of achieving accurate results are investigated.

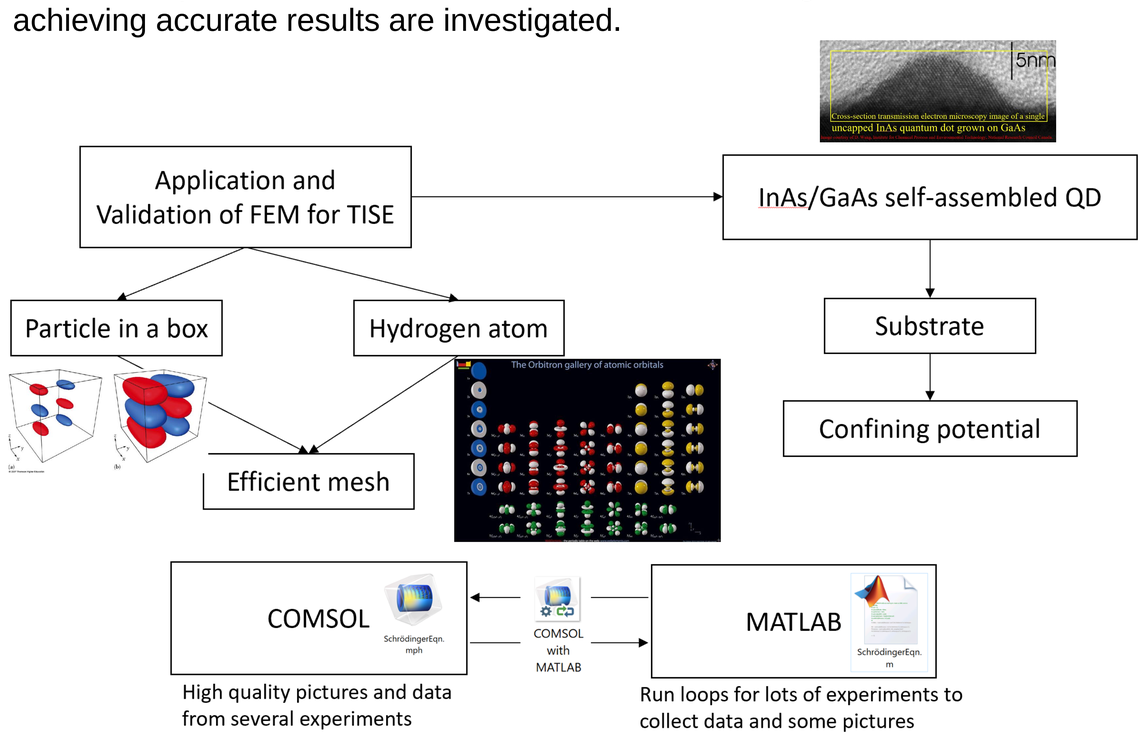


Figure 1: the key framework of the research

COMPUTATIONAL METHODS: We used powerful PDE module and LiveLink™ with MATLAB® in COMSOL Multiphysics®. We solved the Time Independent Schrödinger Equation (TISE) for normalized electron wave functions (EWFs) and corresponding electron energy levels (EELs) for different models[3].

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

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

$$\begin{cases} V_{\text{box}} = 0 \\ V_{\text{atom}} = -\dfrac{e^2}{4\pi\epsilon_0\sqrt{x^2+y^2+z^2}} & \sqrt{x^2+y^2+z^2}\in(0,3] \\ V_{\text{substrate1}} = 0.77 \\ V_{\text{substrate2}} = V(z) = ((-1/800)*z^2 + 0.77) & z\in[0,20] \end{cases}$$

$$m_{\text{box}} = m_{\text{atom}} = m_{\text{e}}$$
$$m_{\text{InAs}} = 0.023 m_{\text{e}}$$
$$m_{\text{GaAs}} = 0.067 m_{\text{e}}$$

mesh1:Lagrange quadratic element, predefined "finer" mesh($e_{\max} = 0.055; e_{\min} = 0.004; e_{\text{mgr}} = 1.4; e_{\text{cf}} = 0.4; e_{\text{ronr}} = 0.7$),Optimization level=High

mesh2:Lagrange quadratic element, predefined "fine" mesh($e_{\max} = 0.055; e_{\min} = 0.004; e_{\text{mgr}} = 1.4; e_{\text{cf}} = 0.4; e_{\text{ronr}} = 0.7$),Optimization level=High, with one defaulted adaptation mesh

mesh3:Lagrange cubic element, predefined "normal" mesh($e_{\max} = 0.055; e_{\min} = 0.004; e_{\text{mgr}} = 1.4; e_{\text{cf}} = 0.4; e_{\text{ronr}} = 0.7$),Optimization level=High

mesh4: Lagrange cubic element, predefined "fine" mesh on top($e_{\max} = 0.08; e_{\min} = 0.01; e_{\text{mgr}} = 1.45; e_{\text{cf}} = 0.5; e_{\text{ronr}} = 0.6$),Swept mesh distribution: the number of layers is 20,Optimization level=High

$$\psi = 0 \qquad \text{on } \partial\Omega$$
$$\vec{n}\cdot\nabla\psi = 0 \qquad \text{on } \partial\Omega$$

element orders	mesh expression
quadratic	$0.154 * sqrt(x^2+y^2+z^2) + 0.01$
cubic	$0.24 * sqrt(x^2+y^2+z^2) + 0.01$

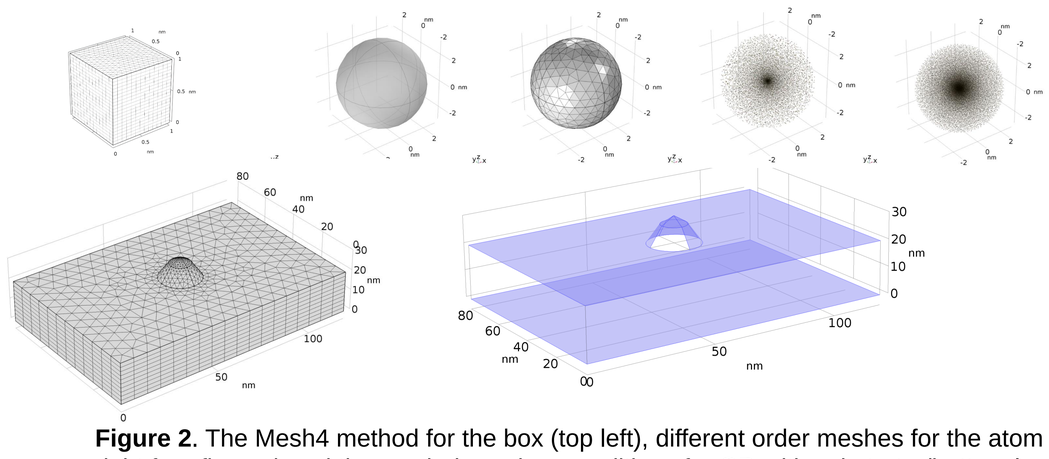
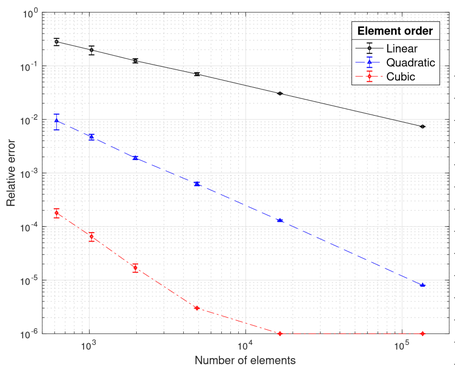


Figure 2. The Mesh4 method for the box (top left), different order meshes for the atom (top right four figures) and the mesh, boundary conditions for QD with substrate (bottom layer)

RESULTS:

mesh methods	DOFs(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}



(n_x, n_y, n_z)	$Deg.$	E_{exact}	Rel_{mesh1}	Rel_{mesh2}	Rel_{mesh3}	Rel_{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

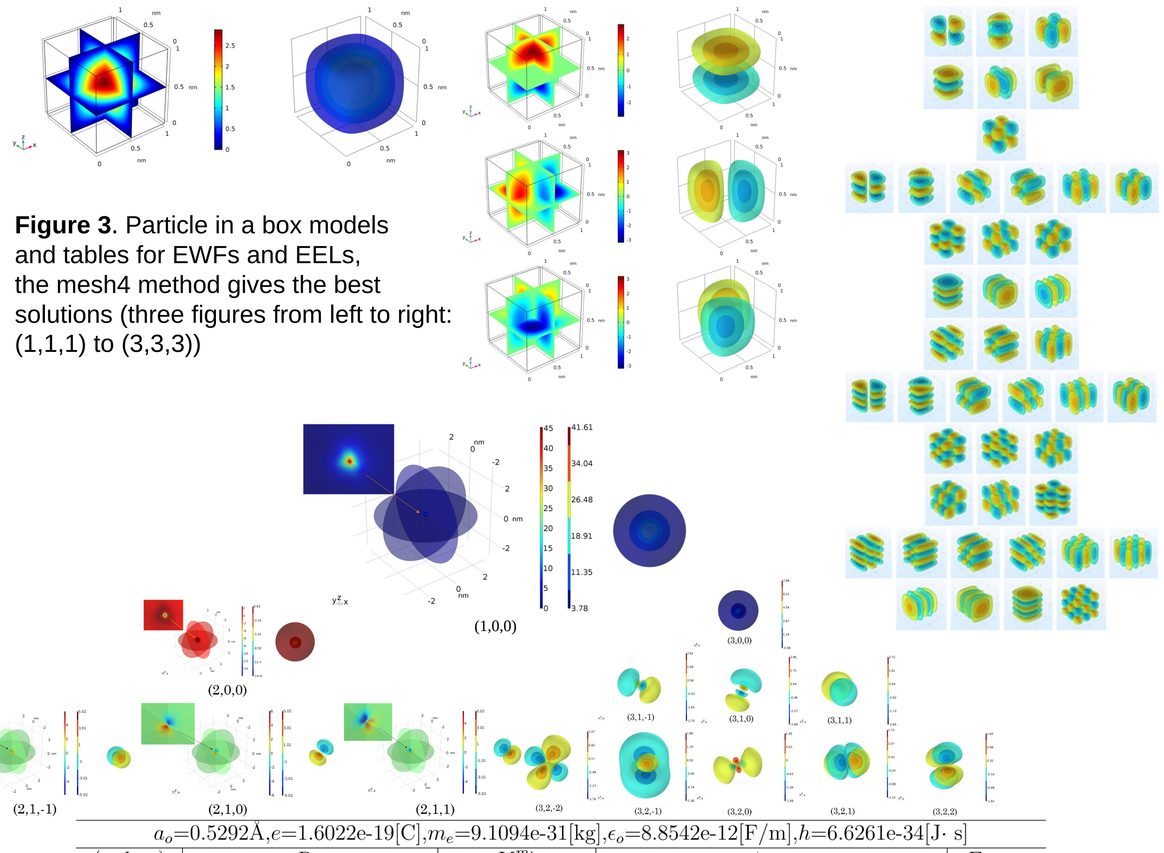


Figure 3. Particle in a box models and tables for EWFs and EELs, the mesh4 method gives the best solutions (three figures from left to right: (1,1,1) to (3,3,3))

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

element orders	mesh expression	No.	DOFs	$E_{(1,0,0)}$	$E_{(2,0,0)}$	$E_{2,1,0}$	$E_{2,1,1}$	$E_{2,1,-1}$
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

Figure 4. Hydrogen atom models and tables for EWFs and EELs, the mesh expression with cubic order elements gives the best solutions (principal quantum number n=1 to n=3)

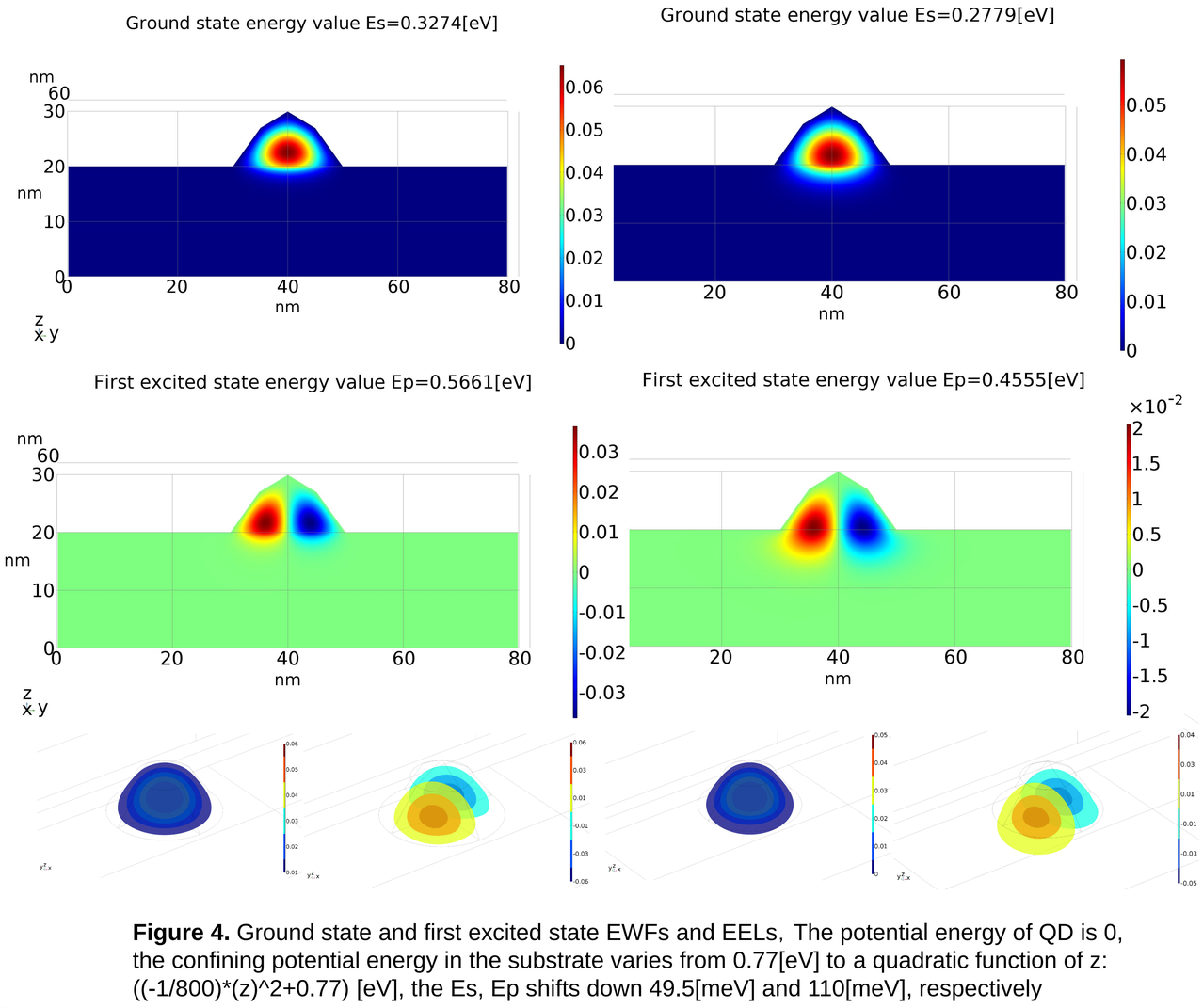


Figure 4. Ground state and first excited state EWFs and EELs, The potential energy of QD is 0, the confining potential energy in the substrate varies from 0.77[eV] to a quadratic function of z: ((-1/800)*(z)^2+0.77) [eV], the Es, Ep shifts down 49.5[meV] and 110[meV], respectively

CONCLUSIONS: The results show that the confining potential of the substrate plays an important role in engineering electron energies as well as wave functions in QDs. Moreover, we have successfully validated the computational approach with known analytical solutions.

REFERENCES:

1. COMSOL Multiphysics Reference Manual, Version 5.3, COMSOL, Inc, www.comsol.com
2. Li, Y., Voskoboynikov, O., Lee, C. P., Sze, S. M., & Tretyak, O. "Effect of shape and size on electron transition energies of InAs semiconductor quantum dots." Japanese journal of applied physics 41(4S),2698(2002).
3. J.Liu and M.Z.Hossain,"Quantum confinement in thin-film alloy quantum dots", (in preparation)

Excerpt from the Proceedings of the 2018 COMSOL Conference in Boston