

Tutorial5A: (real) Device Simulations – Quantum Dots

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Tillmann Kubis, Michael Povolotskyi, Jim

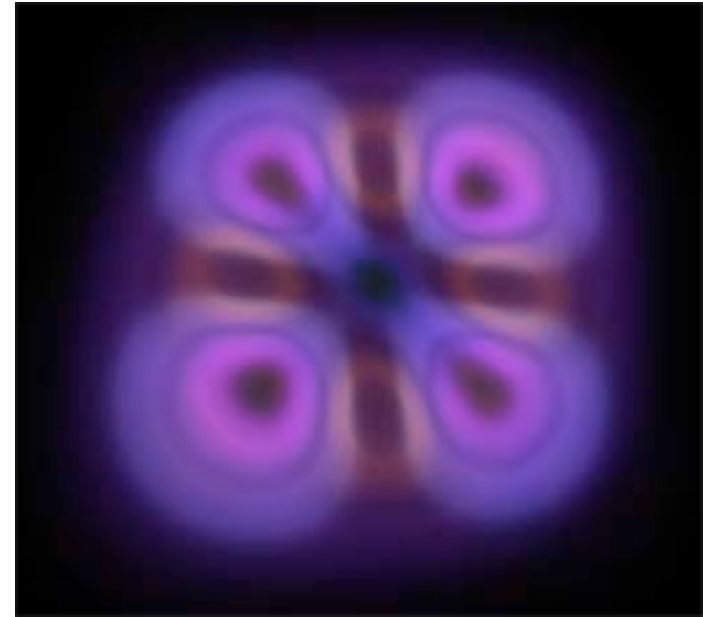
Fonseca, Gerhard Klimeck

Network for Computational Nanotechnology (NCN)

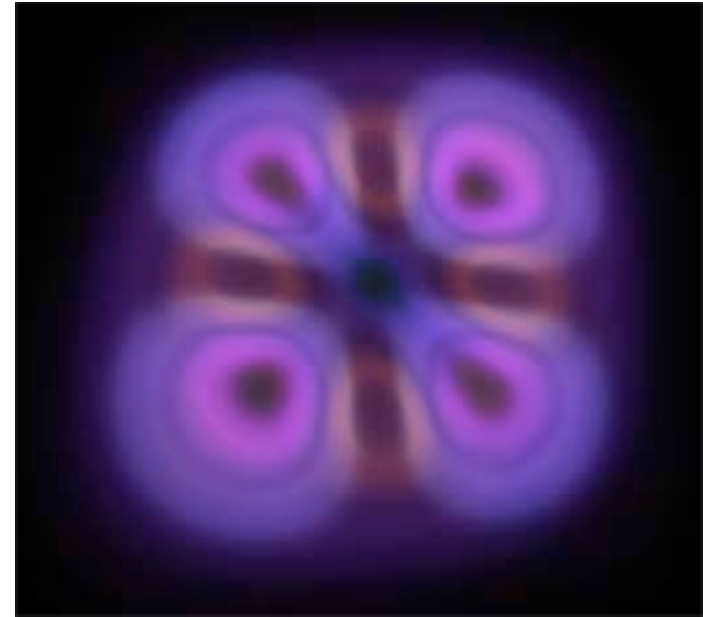
Electrical and Computer Engineering

In this tutorial

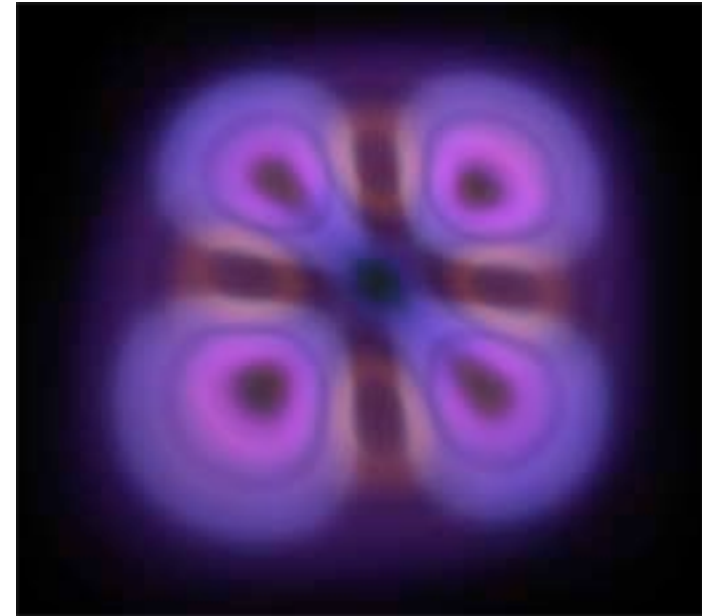
- What is a Quantum Dot?



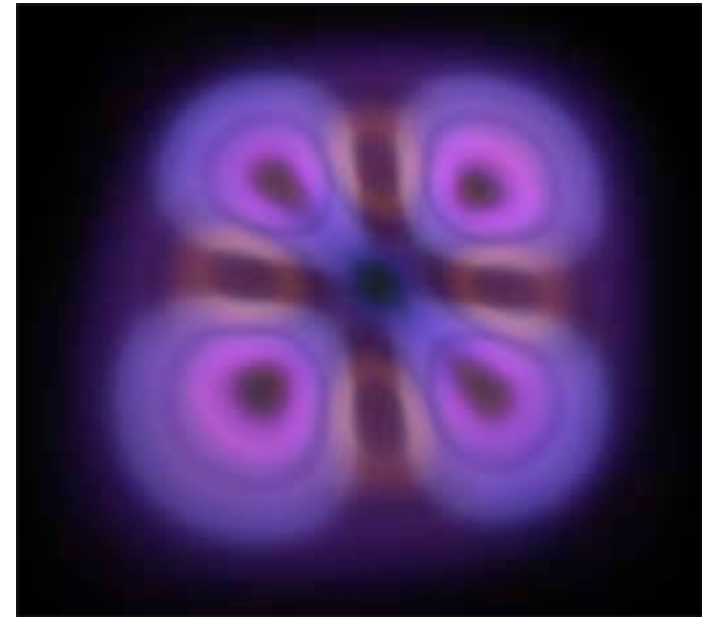
- What is a Quantum Dot?
- What are QDs applications?



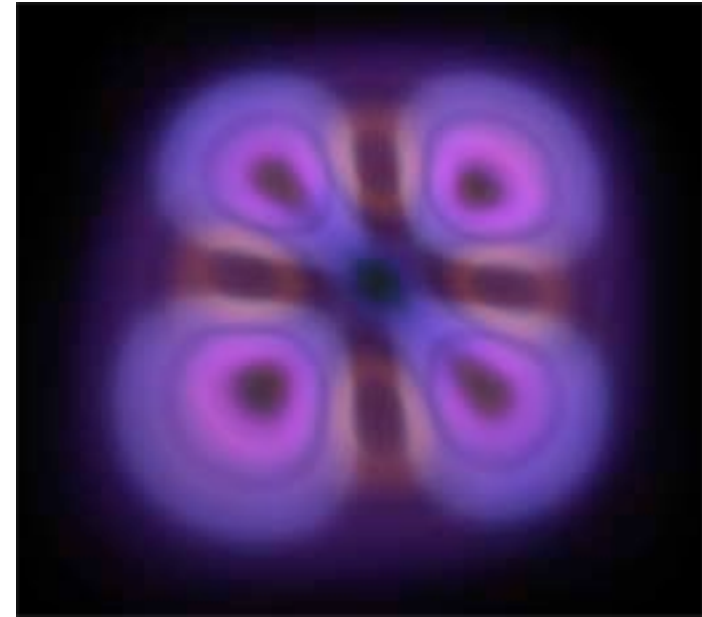
- What is a Quantum Dot?
- What are QDs applications?
- Fabrication of Quantum Dots



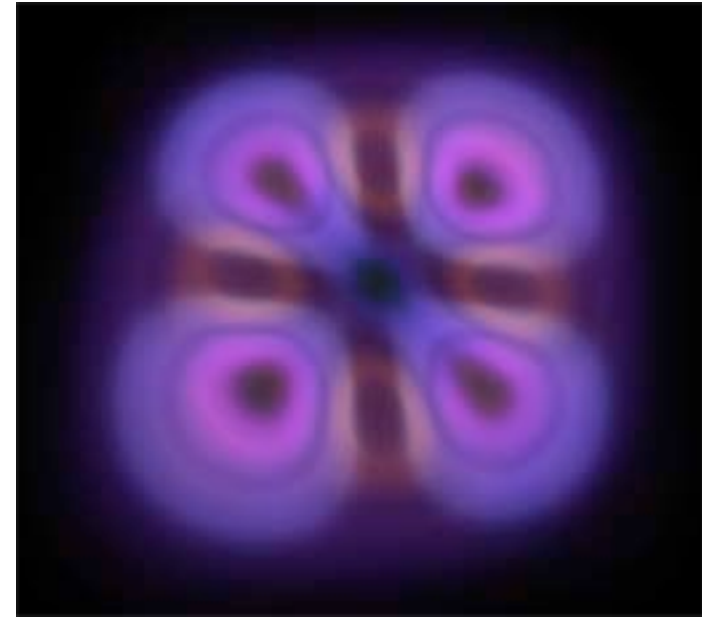
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- Wavefunctions on a subdomain



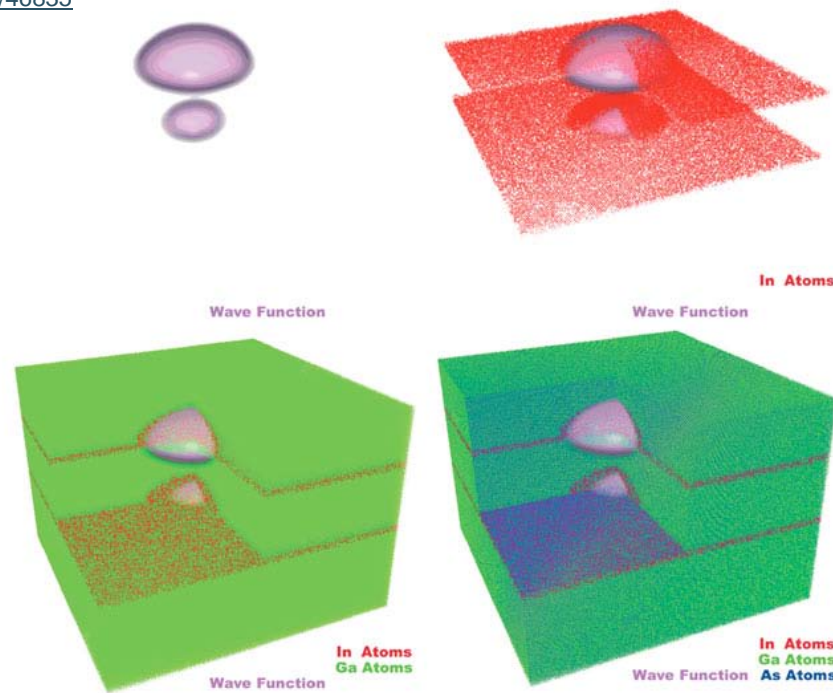
- What is a Quantum Dot?
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- Fabrication of Quantum Dots
- Strain
- Wavefunctions on a subdomain
- Tutorials



What is a Quantum Dot?

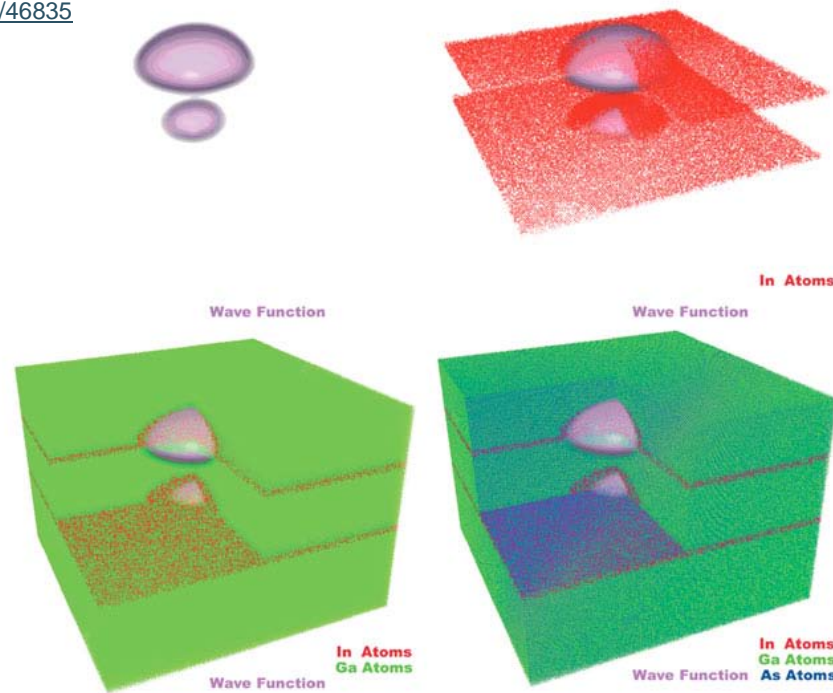
- A quantum dot is a very small portion of matter where carriers are confined.

[8] <http://nanotechweb.org/cws/article/lab/46835>



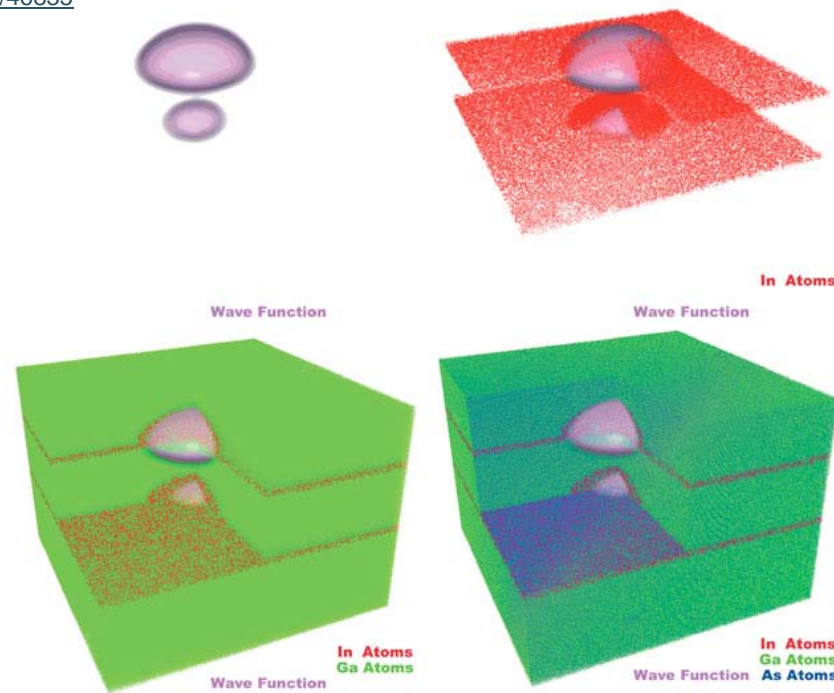
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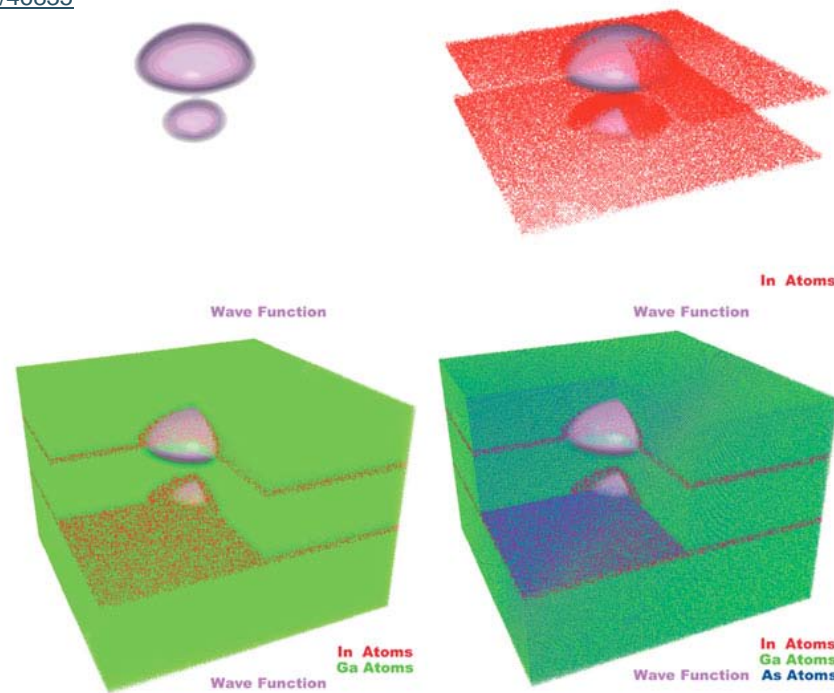
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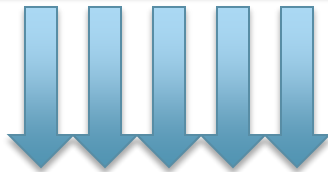
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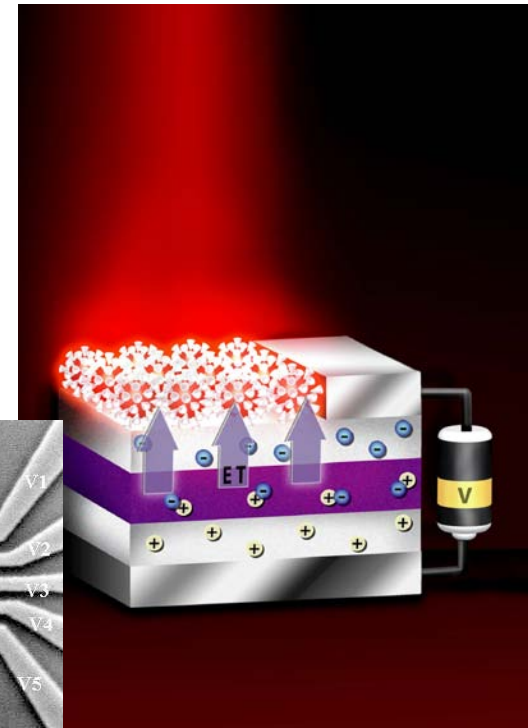
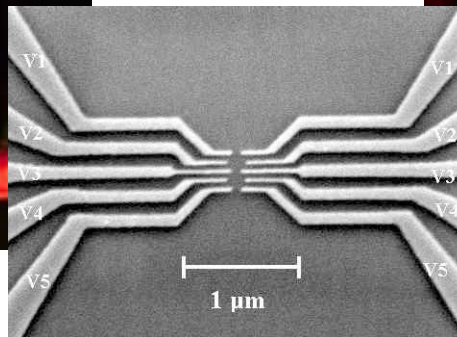
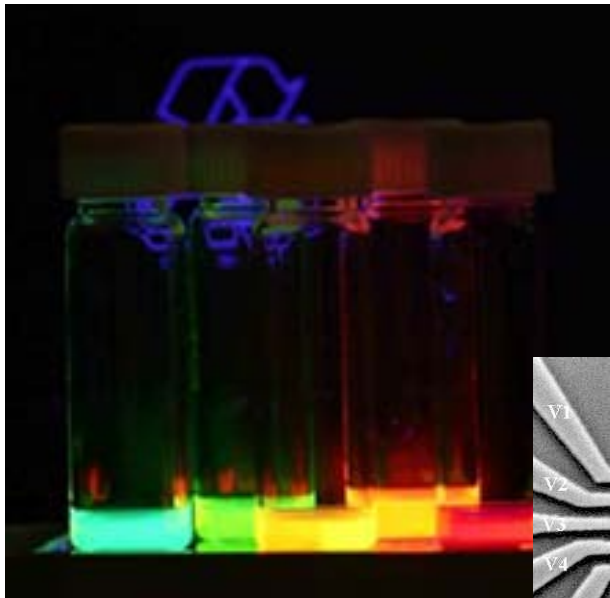
quantum effects are VERY pronounced!

Applications

- QDs are considered to be revolutionary nanoelectronics devices
next-generation lighting, lasers, quantum computing, information storage, quantum cryptography, biological labels, sensors, etc..

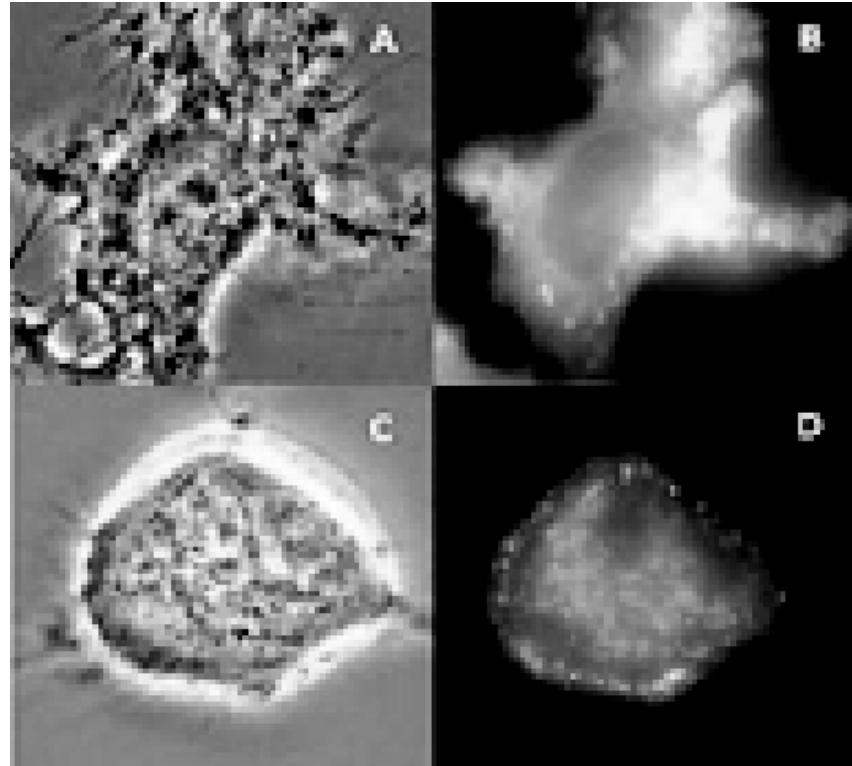
[1] R. Maranganti, P. Sharma, "Handbook of Theoretical and Computational Nanotechnology", American Scientific Publishers.

[3] http://en.wikipedia.org/wiki/Quantum_dot

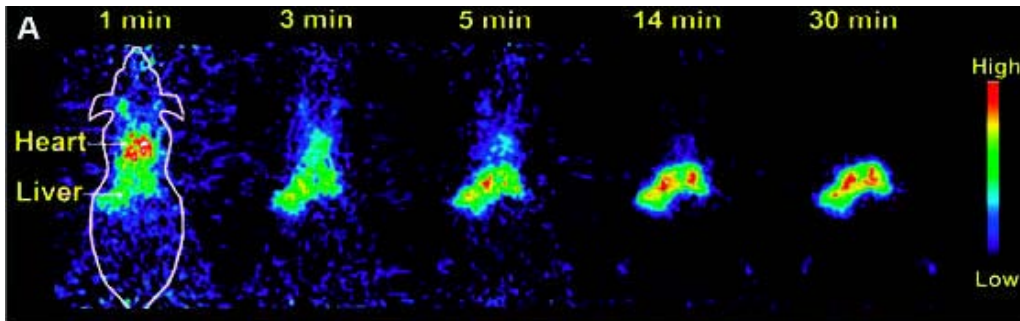


- Magnified view of QD attachment to neurons.

[1] R. Maranganti, P. Sharma,
"Handbook of Theoretical and Computational Nanotechnology",
American Scientific Publishers.

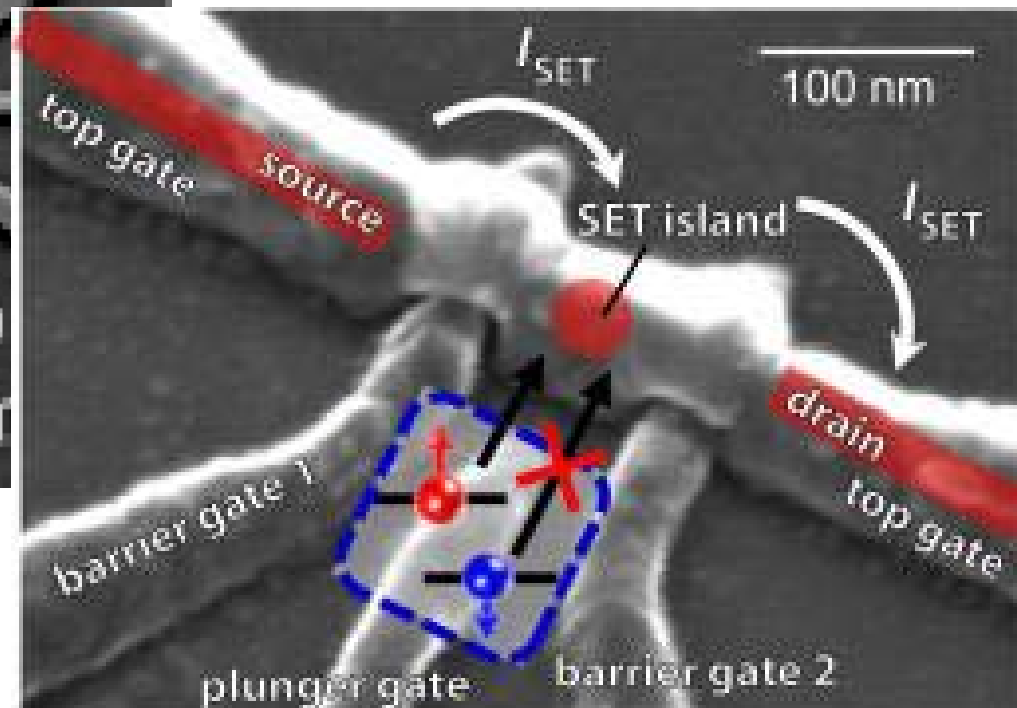
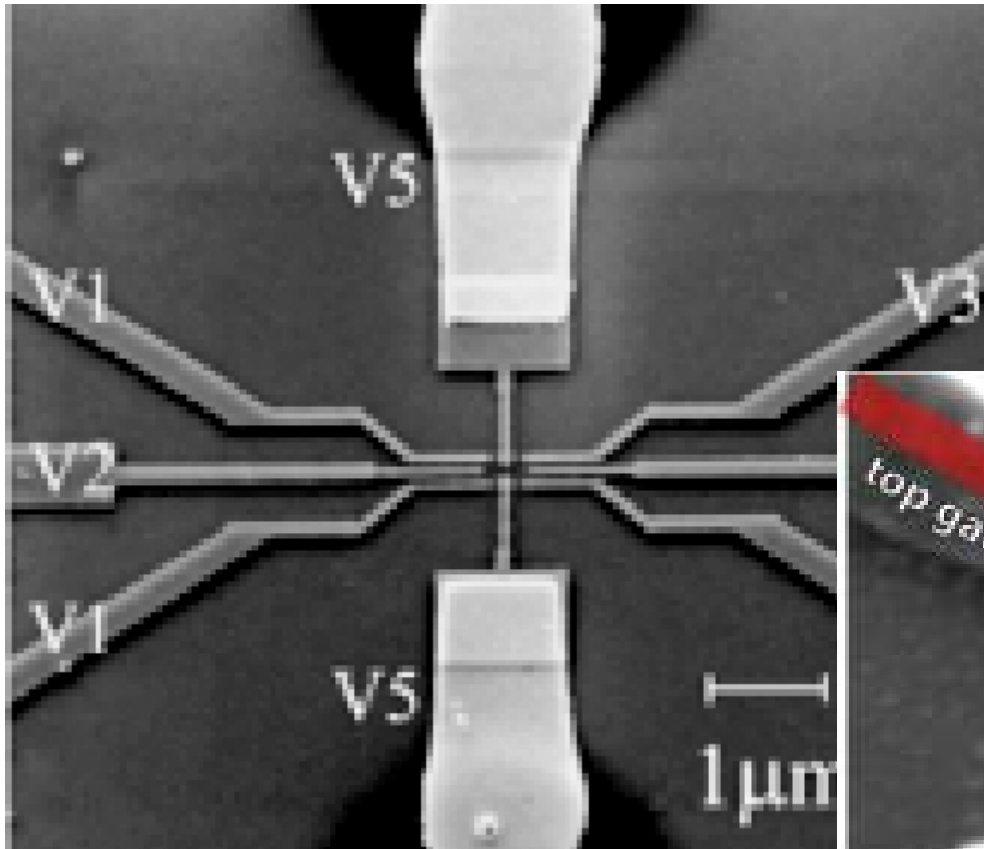


- Tracking of living cells



[4] X. Michalet, et al., "Quantum Dots for Live Cells, in Vivo imaging, and Diagnostics", NIH Public Press.

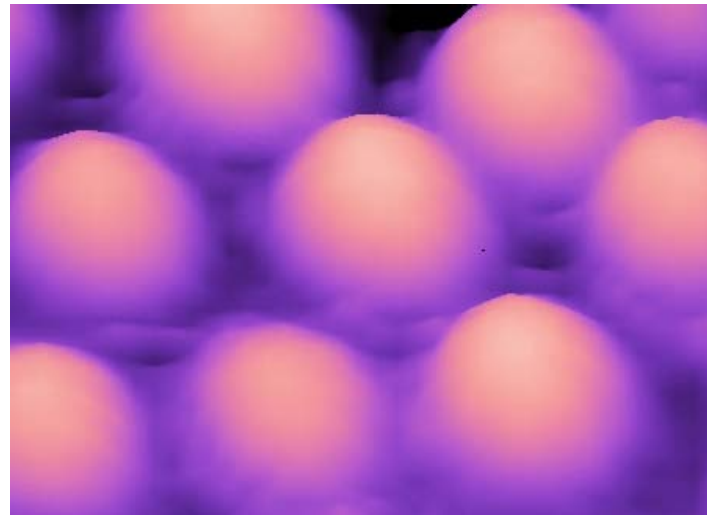
- QD based transistor



[2] Martin Fuechsle, S. Mahapatra, F.A. Zwanenburg, Mark Friesen, M.A. Eriksson, Michelle Y. Simmons, "Spectroscopy of few-electron single-crystal silicon quantum dots", NATURE NANOTECHNOLOGY LETTER.

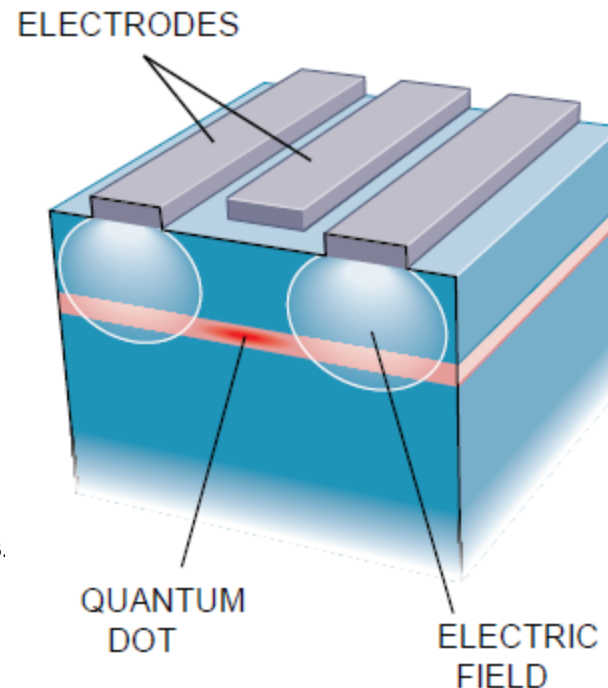
Fabrication

- Strained QDs are:
small regions of materials buried in a larger band gap material
Stranski-Krastanov growth technique



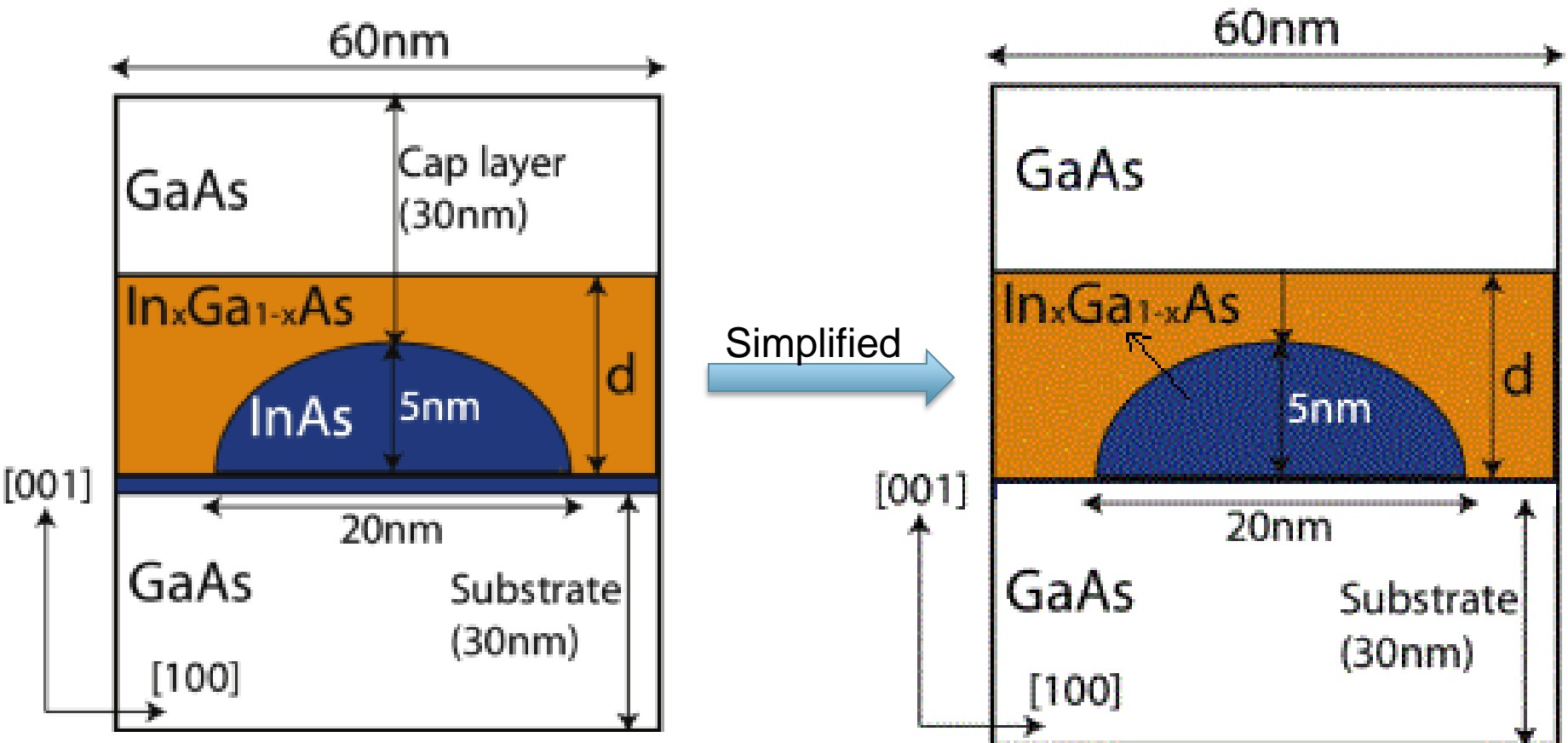
[9] <http://www.kprc.se/Framed/mainWindow.php?id=Doc/QDots.html>

- Electrostatically confined QDs are:
small regions of materials buried in a larger band gap material
built by etching technique



[10] M. Reed, "Quantum Dots", Scientific American, January 1993.

Simulation of Quantum Dots



[5] M. Usman et al., "Moving Toward Nano-TCAD Through Multimillion-Atom Quantum-Dot Simulations Matching Experimental Data", IEEE Transactions on Nanotechnology, Vol. 8, No. 3, May 2009.

- What are the models needed to simulate such structures?

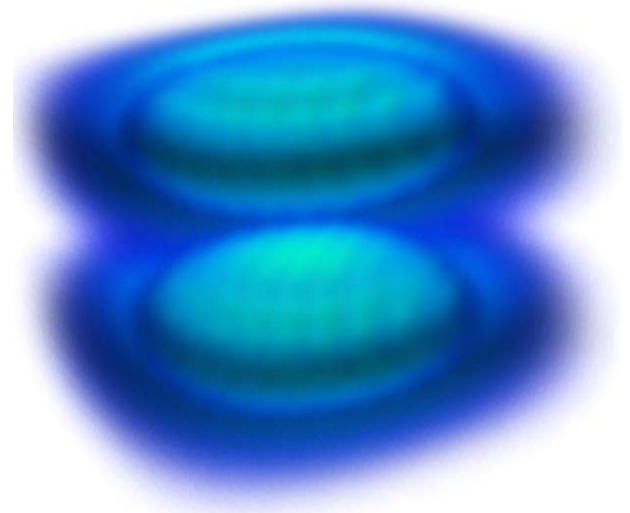
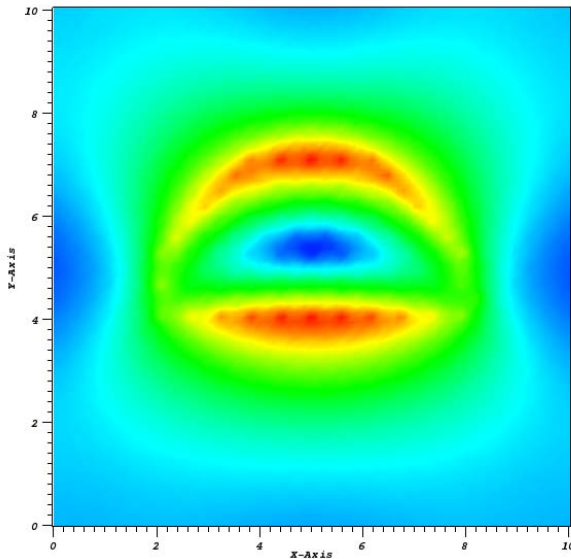
Importance of long range strain effects

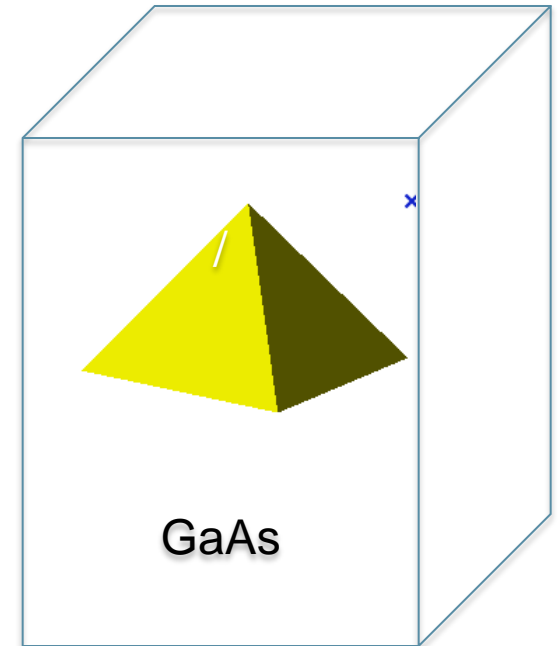
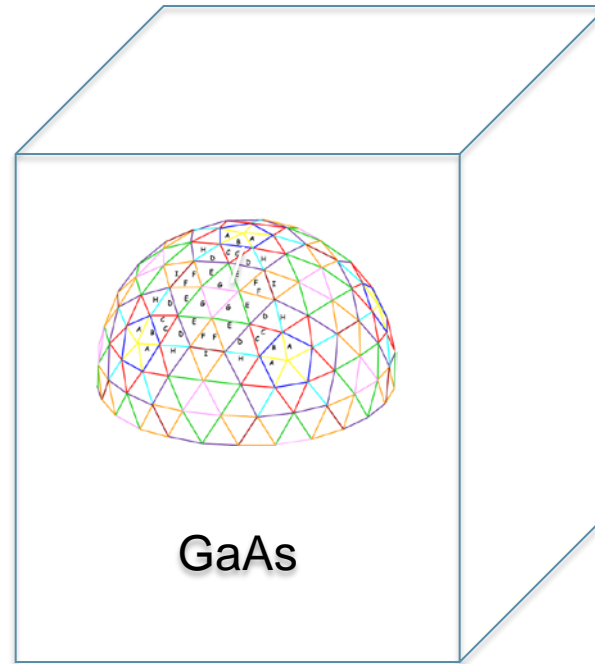
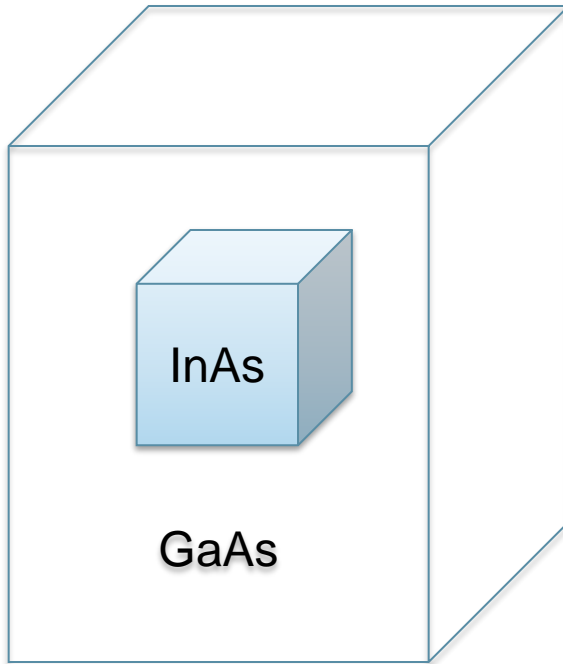
Schroedinger equation in tight-binding formalism

- What are the models needed to simulate such structures?

Importance of long range strain effects

Schroedinger equation in tight-binding formalism





- **shape**

cuboid, spheroid, pyramid, cylinder or dome.

Region

```
{  
  shape          = cuboid  
  region_number  = 3  
  priority       = 1  
  min            = (2.262,0,0)  
  max            = (3.4,1.5,1.5)  
}
```

- Spatial Parallelization (method 1)

Partitioning

```
{  
  x_extension = (-0.5, 24.5)  
  y_extension = (-0.5, 24.5)  
  z_extension = (-0.5, 40.5)  
  num_geom_CPUs = 256  
}
```


- Spatial Parallelization (method 2)

Partitioning

```
{  
  x_partition_nodes = (-1.0 , 4.5, 9, 13.5, 18, 22.5, 27, 31.5, 36)  
  y_partition_nodes = (-1.0 , 4.5, 9, 13.5, 18, 22.5, 27, 31.5, 36)  
  z_partition_nodes = (-1.0 , 4.5, 9, 13.5, 18, 22.5, 27, 31.5, 36)  
}
```

Some words on validation