

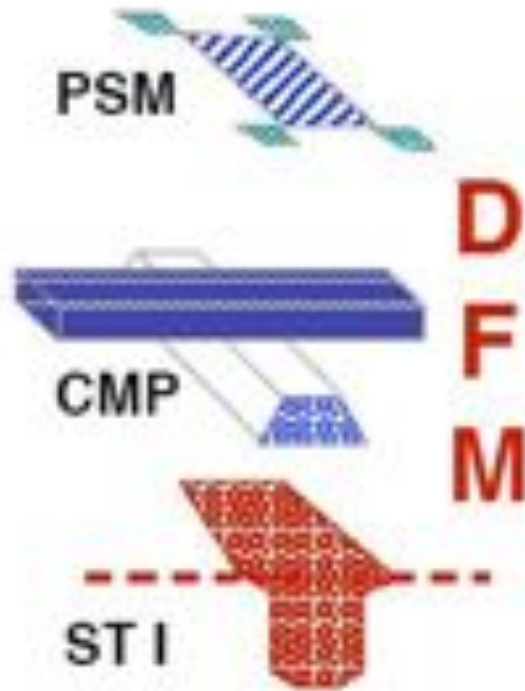
Technology computer aided design (TCAD) of phosphor-free nanowire white LEDs

Kirk H. Bevan & Hong Guo

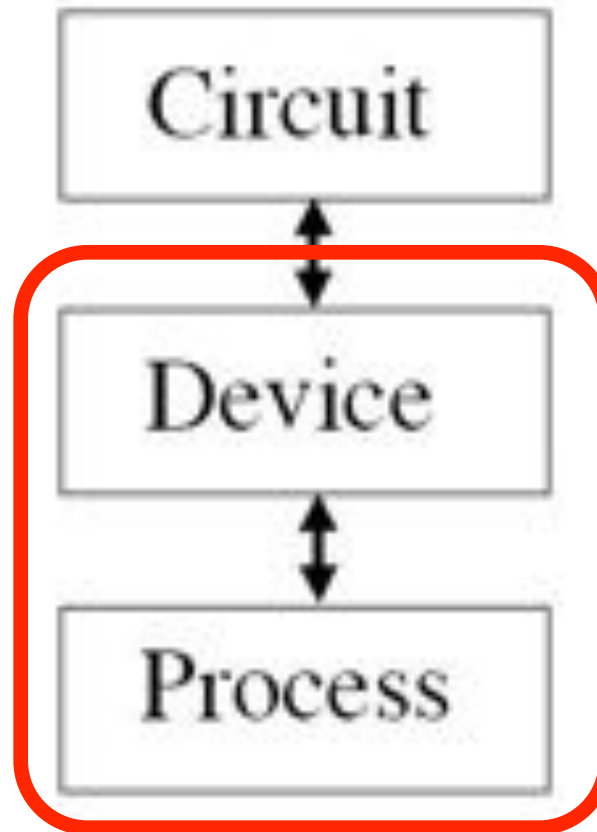


What is TCAD?

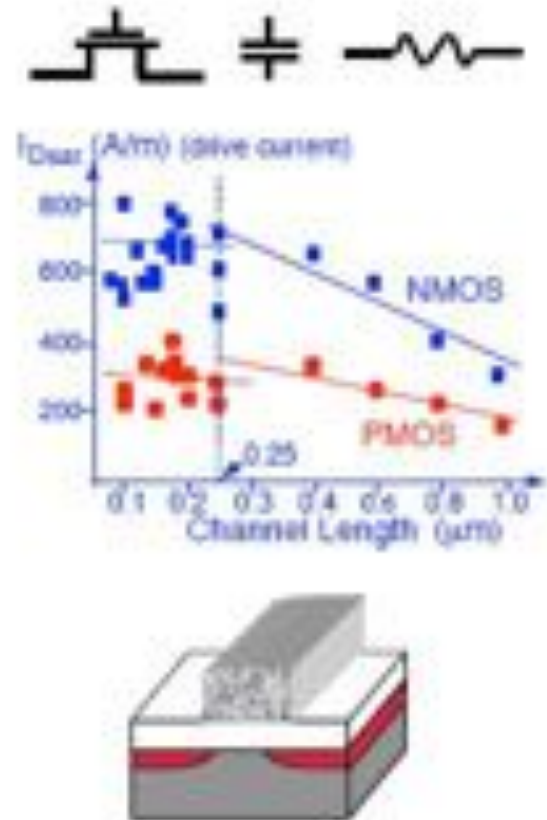
Extrinsic (and Layout)



Intrinsic (active/passive devices)



LEDs



<http://en.wikipedia.org/wiki/File:TCAD-overview.JPG>

- Design for Manufacturing (DFM):
 - Phase Shift Masking (PSM); Chemical & Mechanical Planarization (CMP); Shallow-Trench Isolation (STI).

TCAD Companies & Market Value

SYNOPSYS®

- Yearly Revenues: ~1.5 Billion
- Employees: ~7000



SILVACO

- Yearly Revenues: ~10 Million
- Employees: ~250



COMSOL

- Yearly Revenues: Undisclosed
- Employees: ~250



CROSLIGHT

Software Inc.

- Yearly Revenues: Undisclosed
- Employees: ~25



NanoAcademic Technologies

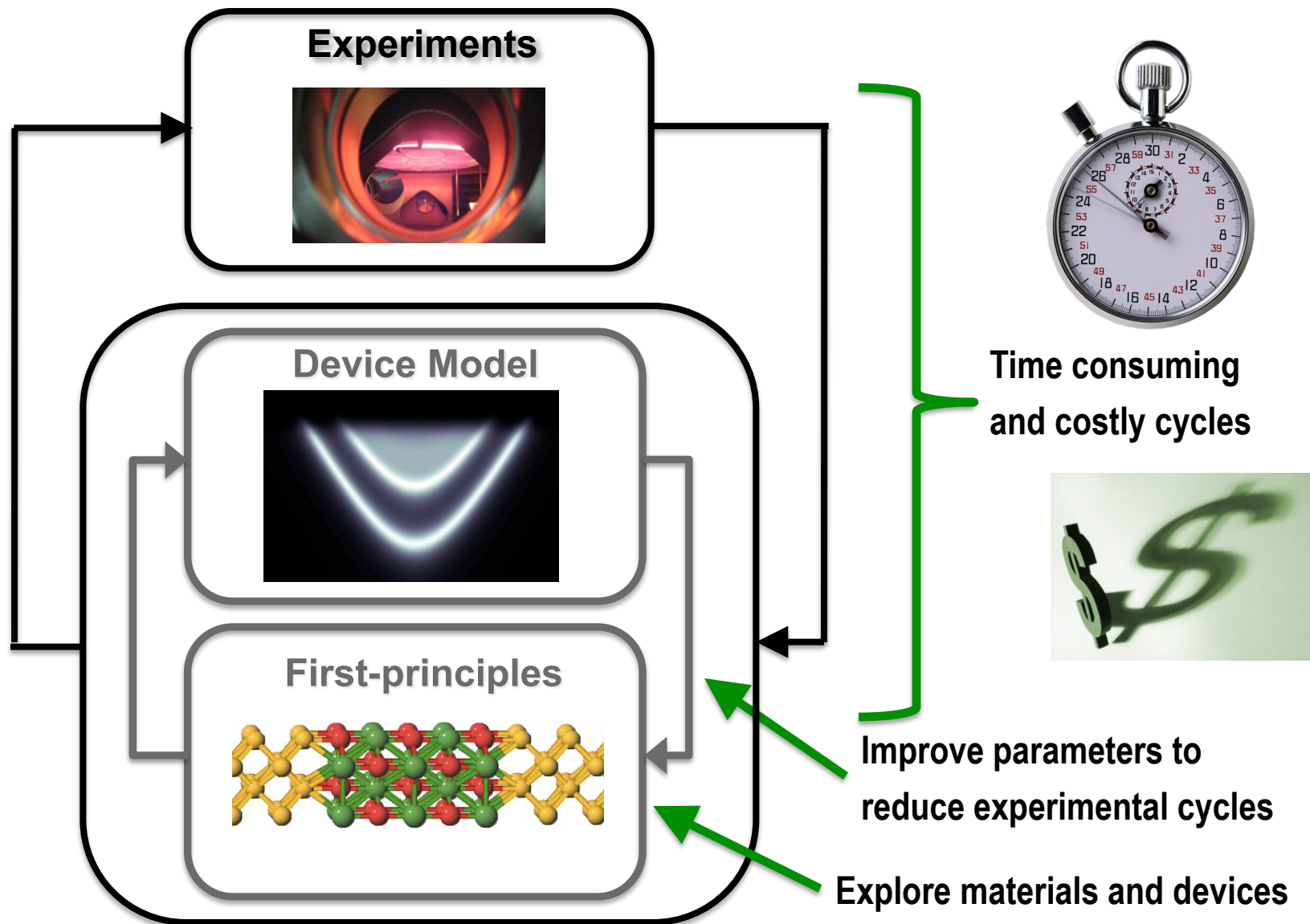
Software Tools for Nanoelectronics

- Yearly Revenues: Undisclosed
- Employees: ~5



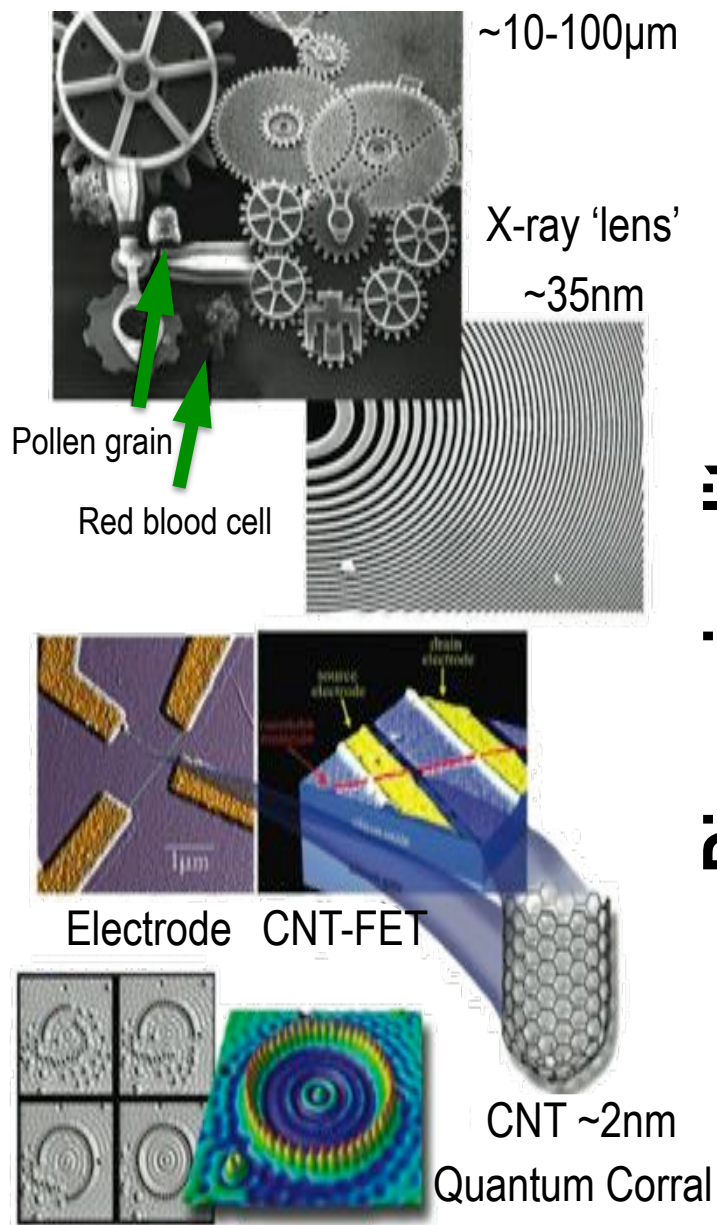
Large Market Room For Growth

Why Use TCAD?



http://cio.gsfc.nasa.gov/centers/jpl/images/content/352556main_wafer-20090528-browse.jpg

TCAD Hierarchy



Dimensionality

Model Parameters

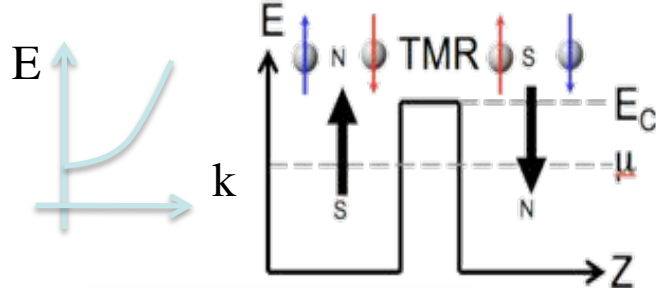
$$E = \frac{\hbar^2 k^2}{2m^*}$$

$$E_{C,t_0}$$

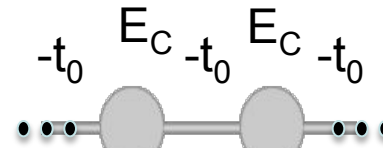
$$V_{XC} = Cn(\vec{r})^{1/3}$$

$$C = \frac{-3}{4(3/\pi)^{1/3}}$$

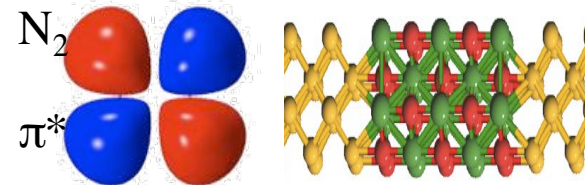
Effective Mass



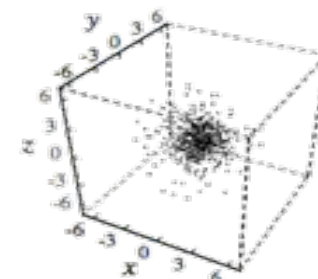
Tight binding



First-principles



Quantum Monte Carlo



Design Requirements

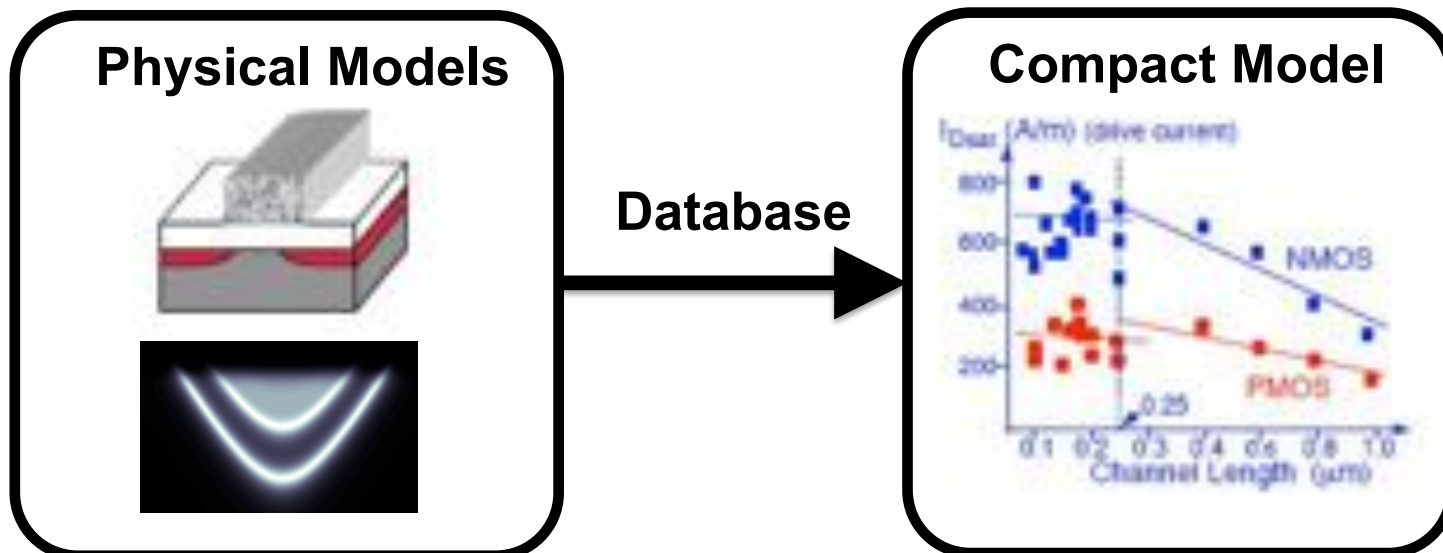
TCAD Theme

■ Proposed Projects:

1. Engineering Enhanced P-type Doping in InGaN/GaN
2. Optimizing InGaN/GaN Nanowire Morphology and Growth
3. Tailoring Carrier Transport and Optical Emission in InGaN/GaN Nanowire LEDs
4. Integrated Compact Nanowire LED Simulator

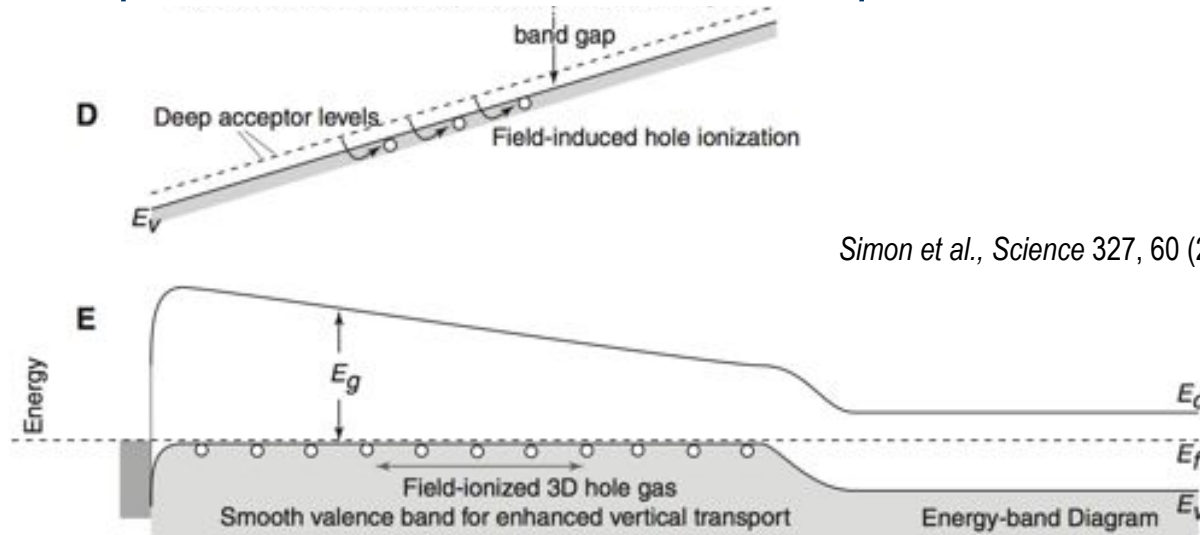
Physical Models

Compact Model

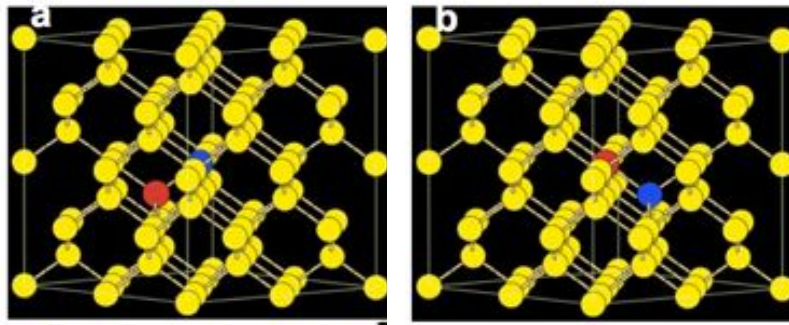


Project 1: Enhanced P-type Doping

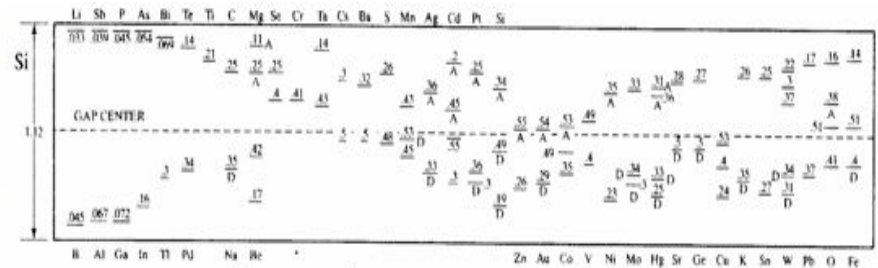
- Hole Injection is a big problem...
 - Task A: Explore Polarization Induced Acceptor Ionization



- Task B: Explore Alternate Dopants



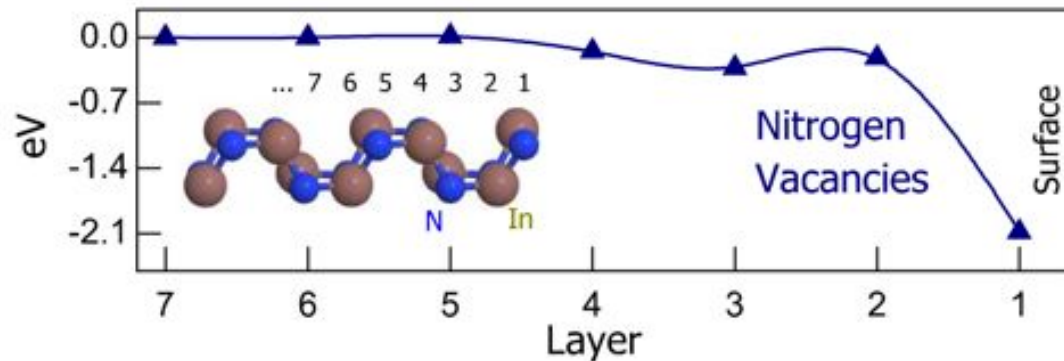
Chen et al., Phys. Rev B 79, 235202 (2009).



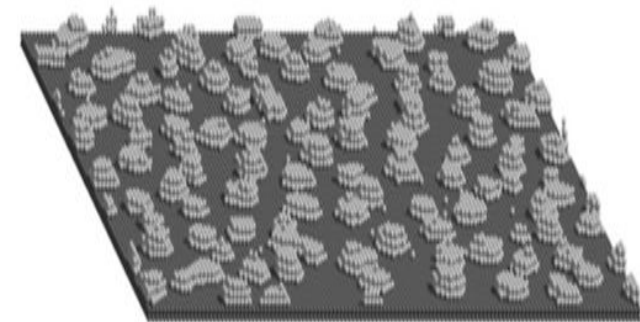
Pierret, "Advanced Semiconductor Fundamentals"

Project 2: Morphology & Growth

- Defects are a major bottleneck...
 - Task A: Reducing Defect Formation During Growth

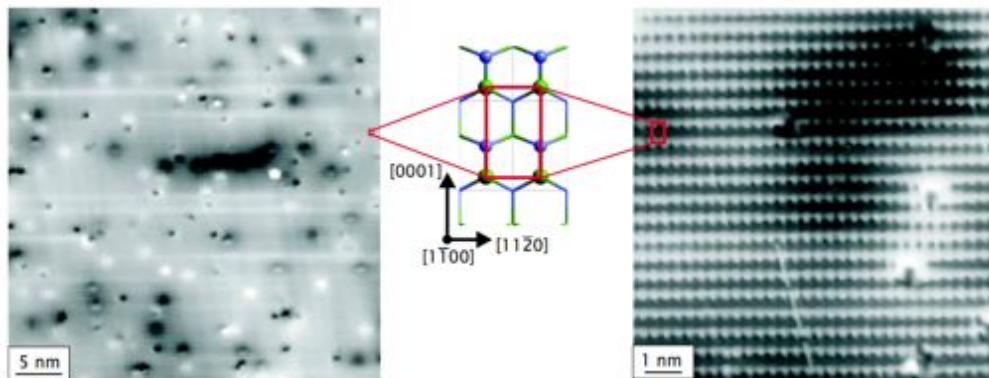


Zhao et al., Nano Lett. 12, 2877 (2012).

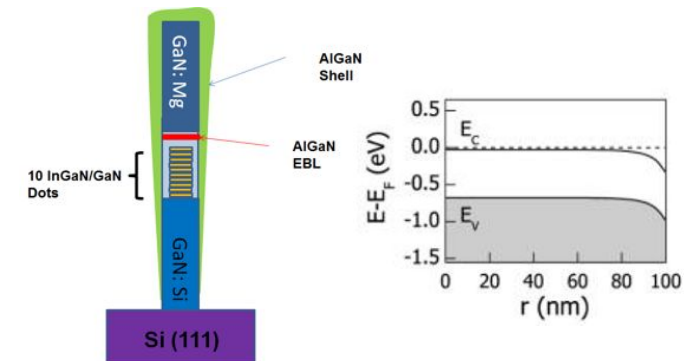


Battaille, Appl. Mech. Engrg., 197, 3386 (2008).

- Task B: Engineering Surface Morphology

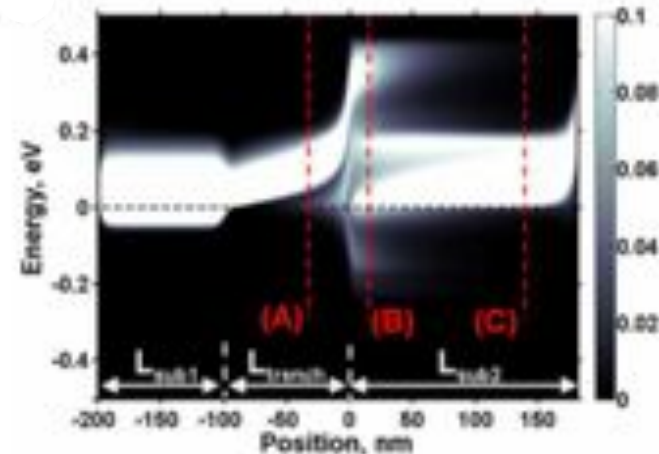
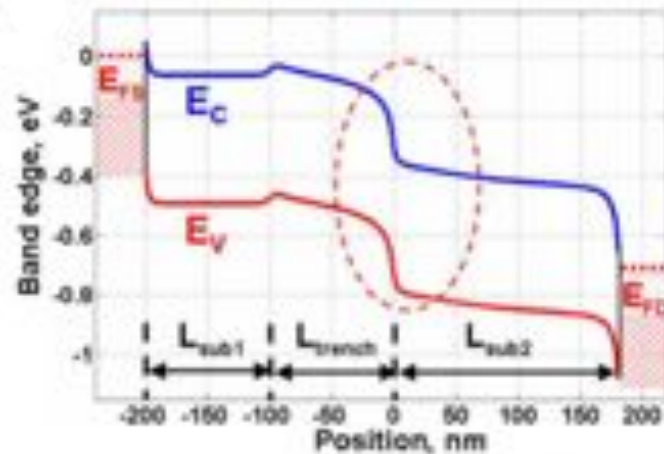


Bertelli et al., Phys. Rev. B 80, 115324 (2012).



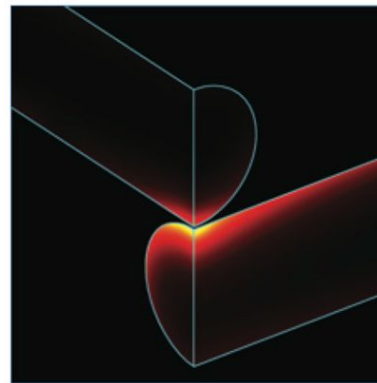
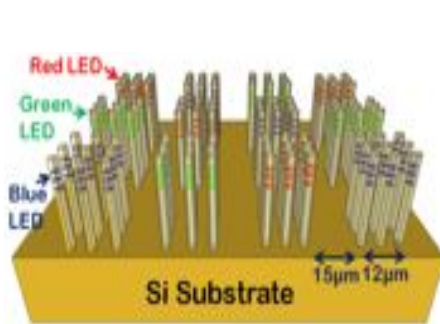
Project 3: Active Device Modeling

- Carrier transport and optical emission...
 - Task A: Optimizing Carrier Transport and Optical Emission



*Koswattta et. al.,
Nano Lett. 8, 1596 (2008)*

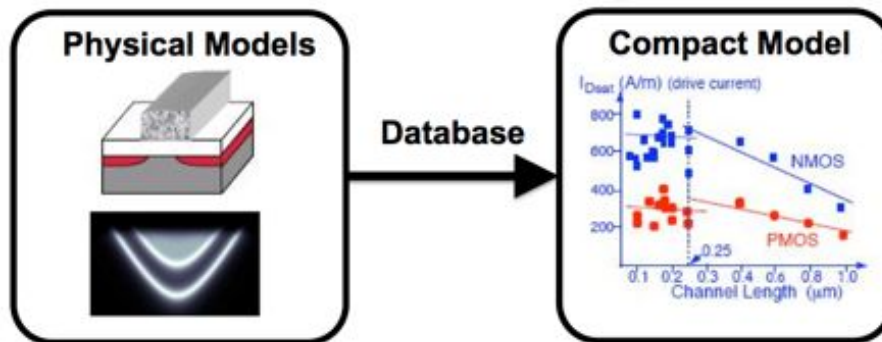
- Task B: Engineering Optical Field Propagation



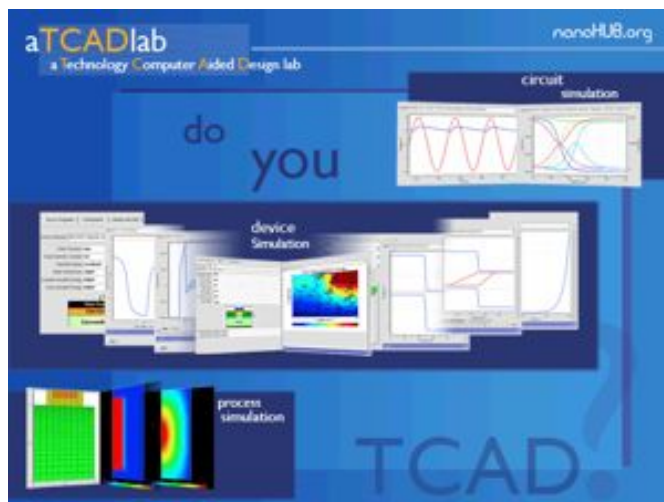
Garnett et. al., Nature Materials 11, 241 (2012)

Project 4: Compact Simulator Hub

- Integrating physical models with partner themes...
 - Task A: Physical Model Database Generation



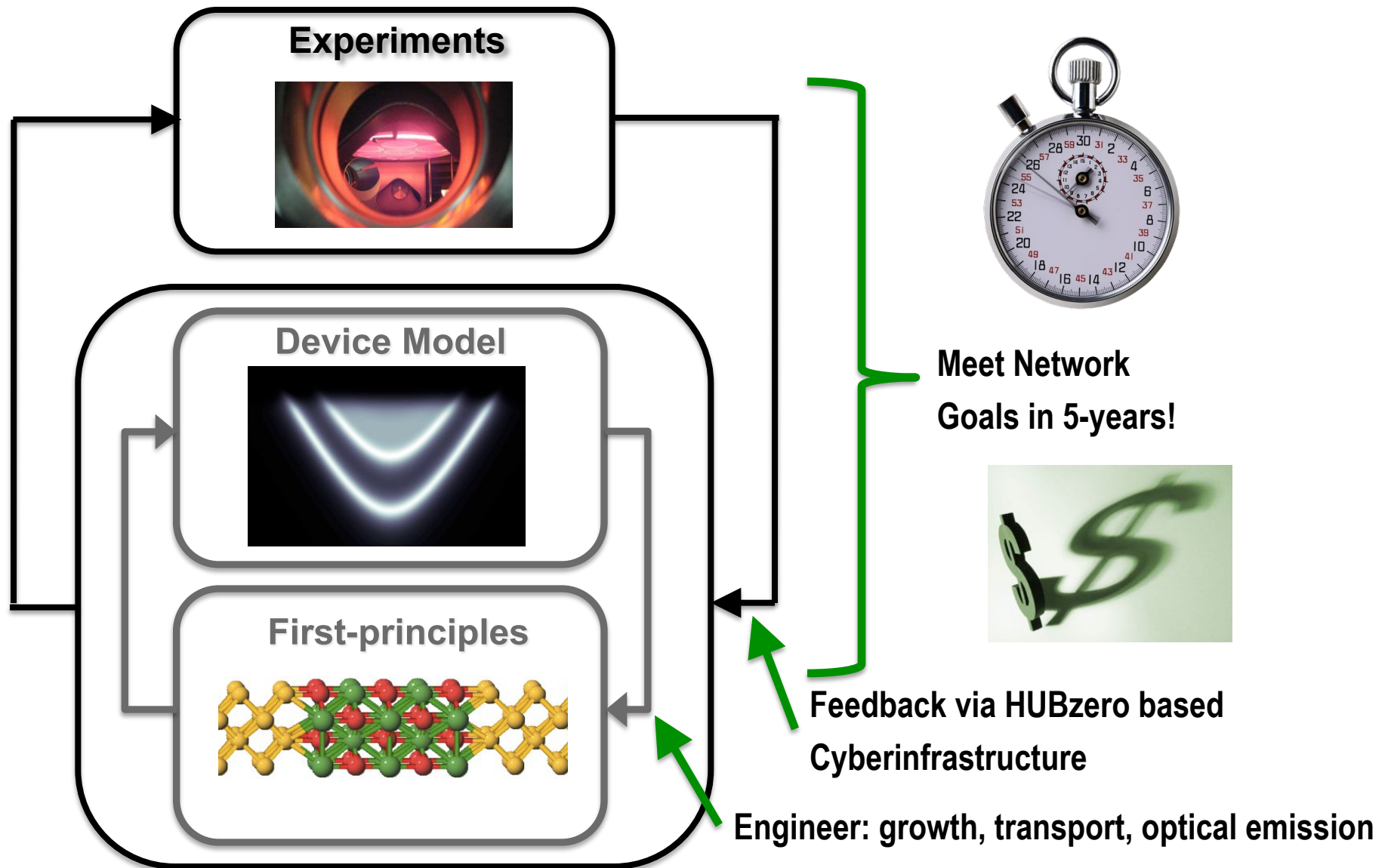
- Task B: Cyberinfrastructure Compact Model Hub



www.hubzero.org

<http://nanohub.org/topics/aTCADLab>

TCAD in the SSL Network



http://cio.gsfc.nasa.gov/centers/jpl/images/content/352556main_wafer-20090528-browse.jpg