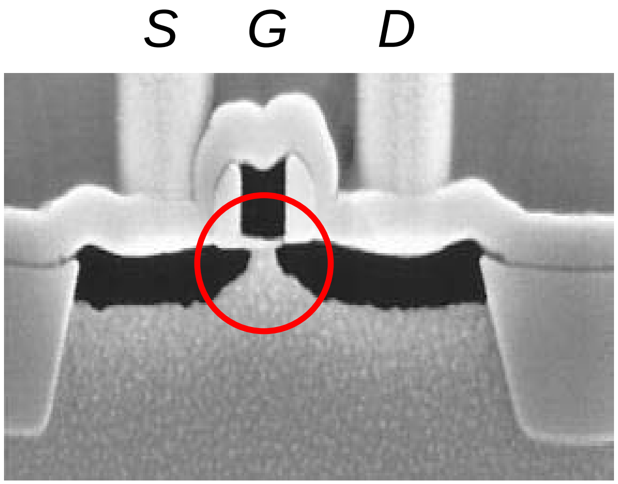
AINE Kickoff, April 4, 2008

# Computational Nanoelectronics in the 21st Century:

## *Challenges and Opportunities*

Mark Lundstrom
Network for Computational Nanotechnology
Purdue University
West Lafayette, IN

# trends in electronic devices



The Silicon MOSFET

**1977:** *L* ~ 5 micrometers (5000 nm)

**2008:** *L* ~ 0.05 micrometers (50 nm)

**Transistors per chip:**

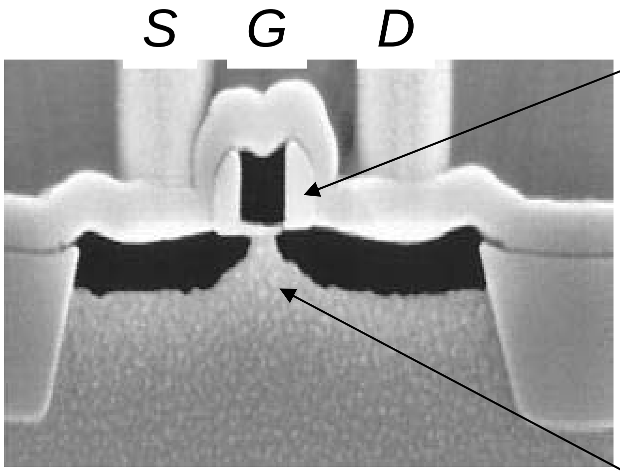
< 10,000 ⌫ > 1,000,000,000

# Challenges for computational electronics

1) Device simulation must address a broader range of problems
2) Simulations must capture quantum and atomic scale effects
3) Computationalists and experimentalists must work together
4) Problem-solving and invention should be emphasized
5) Current tools must evolve and new tools may be necessary
6) Development of new codes must be accelerated

1999 Nanotransistor Meeting, NIST, Gathersberg, Md.

# new materials



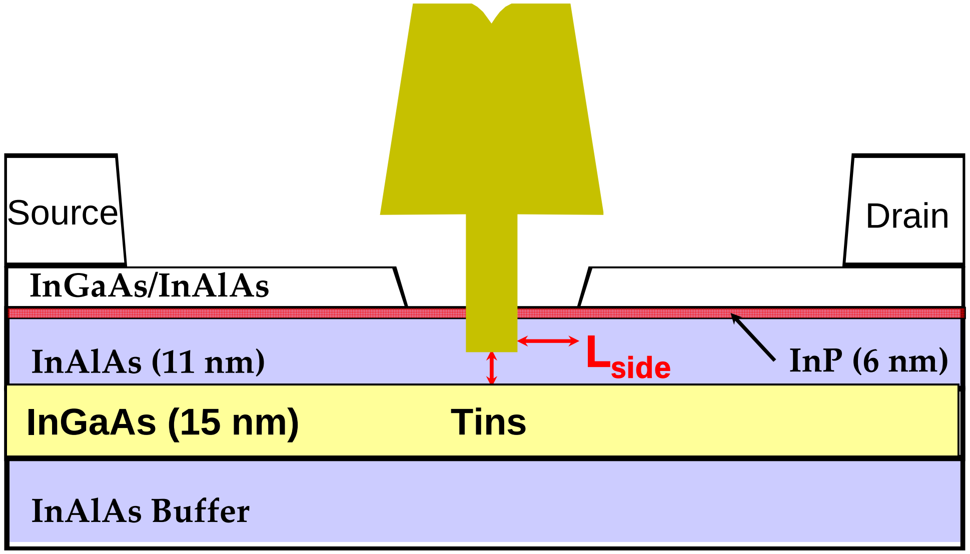
The Silicon MOSFET

45 nm technology

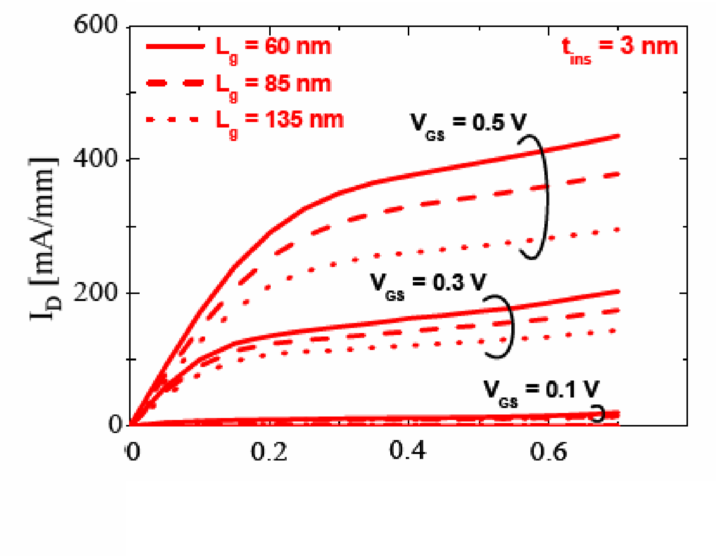
$HfO_2$ + metal gate

Si --> III-V?

# del Alamo group HEMTs



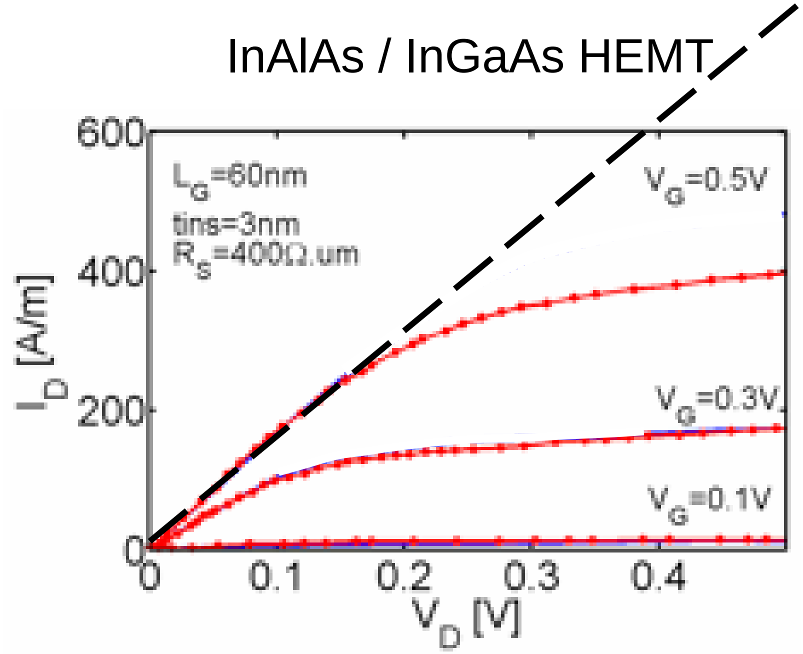
Reference: Dae-Hyun Kim et al. IEDM 2006



Typical $I_{DS}$ vs. $V_{DS}$

# mobility in nanoscale FETs

InAlAs / InGaAs HEMT



Dae-Hyun Kim et al. IEDM 2006

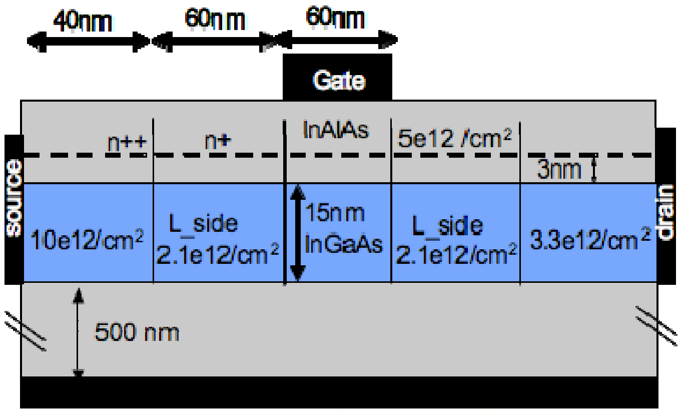
$$I_D = \frac{W}{L}\mu_{eff}C_{ox}\left(V_{GS} - V_T\right)V_{DS}$$

$$\frac{V_{DS}}{I_{DS}} = R_{SD} + \frac{L}{\mu_{eff}C_{ins}(V_G - V_T)}$$

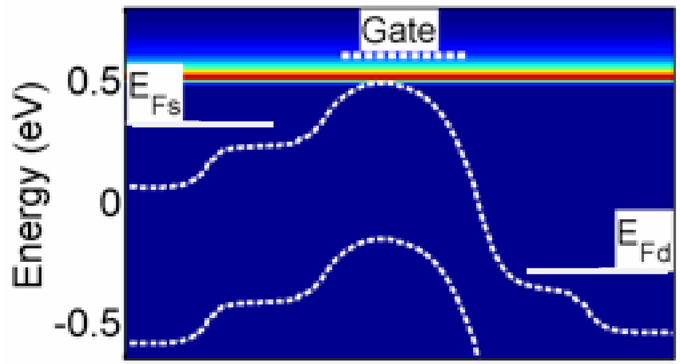
$$\mu_{eff} \approx 170 \text{ cm}^2/\text{V-s}$$

$$\left(\mu_n \approx 10{,}000 \text{ cm}^2/\text{V-s}\right)$$

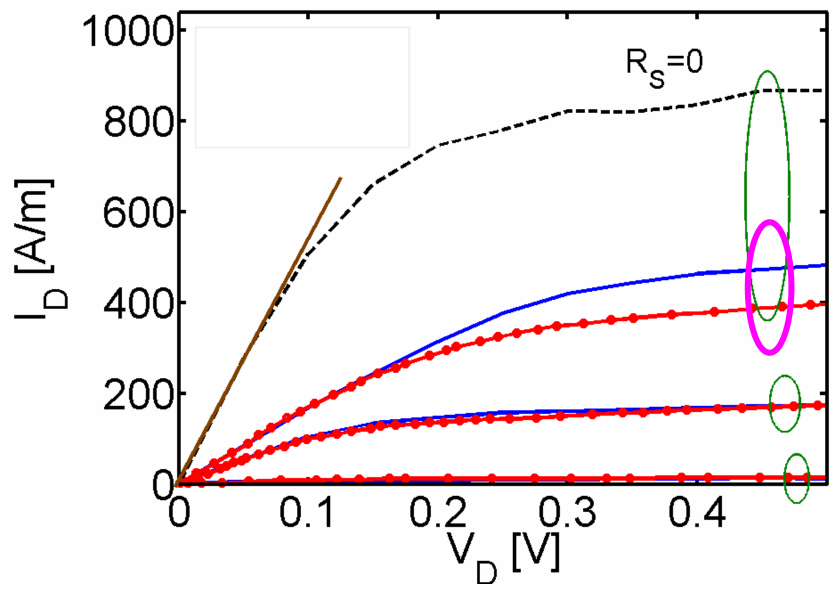
# ballistic IV (Neophytous Neophytou, Purdue)



idealized device structure



2D, real space
NEGF simulation
(eff. mass)



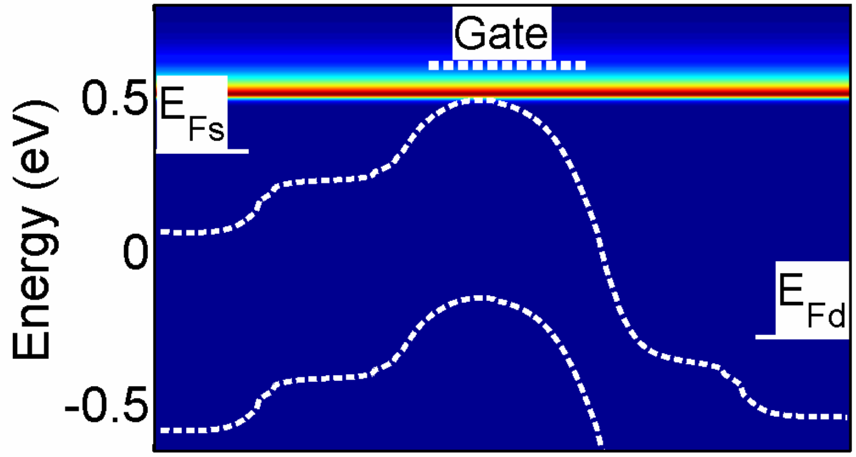
- - - ballistic simulation

— measured
($T_{ins}$ = 3 nm, $L$ = 60 nm)

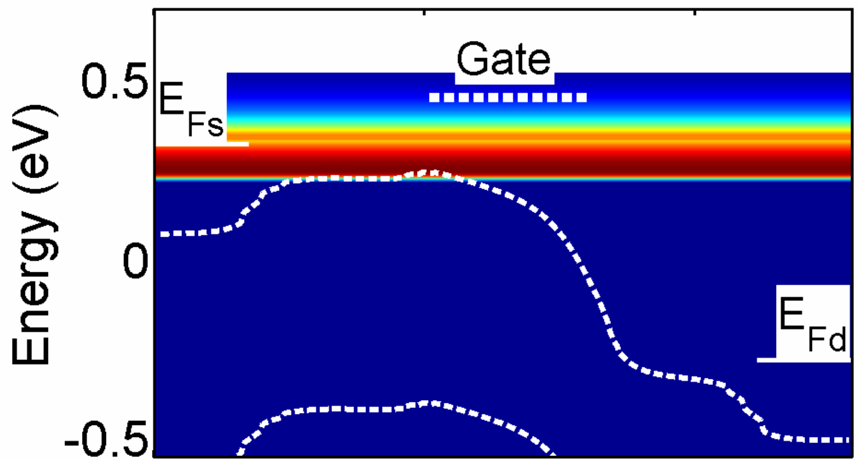
***intrinsic, ballistic FET with external series resistance***

# “source exhaustion”

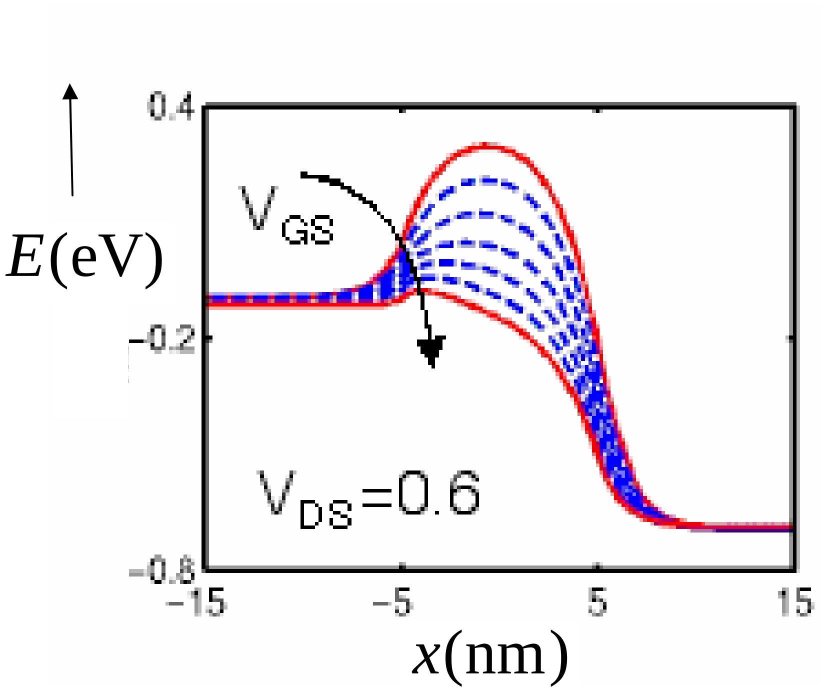
1) OFF state



2) Barrier collapses



# limits of transistors



**Limits**

$$E_S\big|_{\min} = \ln(2)\, k_B T$$

$$L_{\min} \approx \hbar \Big/ \sqrt{2 m E_S\big|_{\min}}$$

$$\tau_{\min} \approx \hbar \Big/ E_S\big|_{\min}$$

$$(\Delta p \Delta x = \hbar)$$

$$(\Delta E\, \Delta t = \hbar)$$

NCN

www.nanoHUB.org

# 45 nm technology vs. limits

## Limits

$$E_S\big|_{\min} = \ln(2)k_BT \approx 0.003 \text{ aJ}$$

$$L_{\min} \approx h\big/\sqrt{2m^*E_{\min}} = 1.5\,\text{nm}\,(300\text{K})$$

$$\tau_{\min} \approx \hbar\big/E_S\big|_{\min} = 0.04\text{ ps} \quad (300\text{K})$$

$$n_{\max}(\text{at }100\text{W/cm}^2) = 1.5\text{ B/cm}^2$$

## 45 nm node

(ITRS 2006 ed.)

$$E_S \approx 5{,}000 \times E_S\big|_{\min}$$

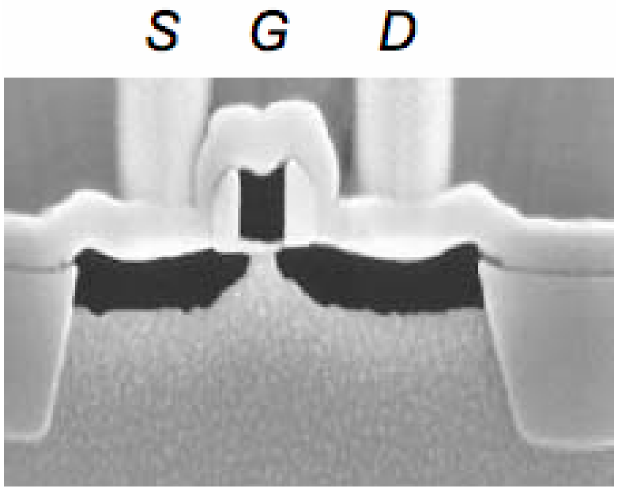
$$L \approx 20 \times L_{\min}$$

$$\tau \approx 20 \times \tau_{\min}$$

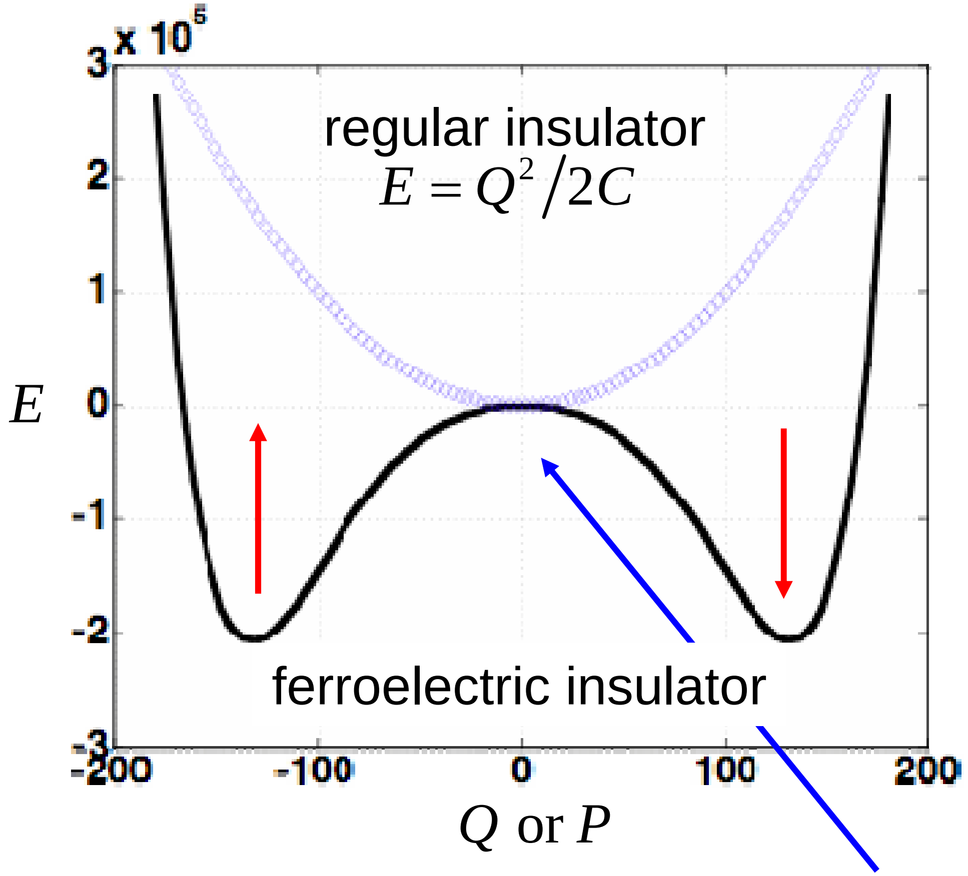
$$n \approx 1\text{ B/cm}^2$$

# the real challenges

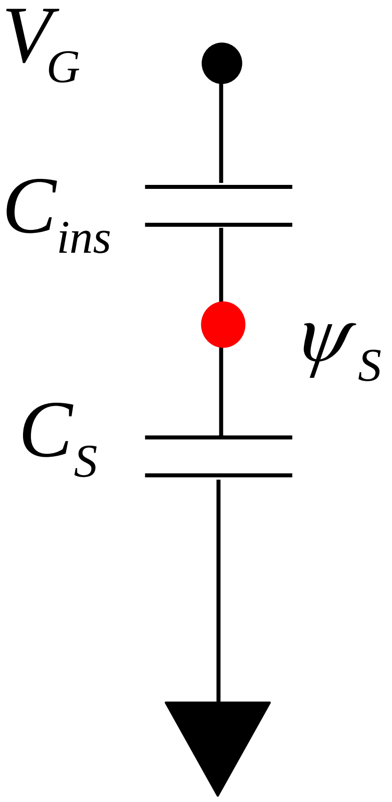
1) electrostatics
2) series resistance
3) parasitic *C*
4) variations
5) voltage scaling



# new ideas?



**negative capacitance!**



$$m = \frac{\partial \mathbf{V}_G}{\partial \psi_S} = 1 + \frac{C_S}{C_{ins}}$$

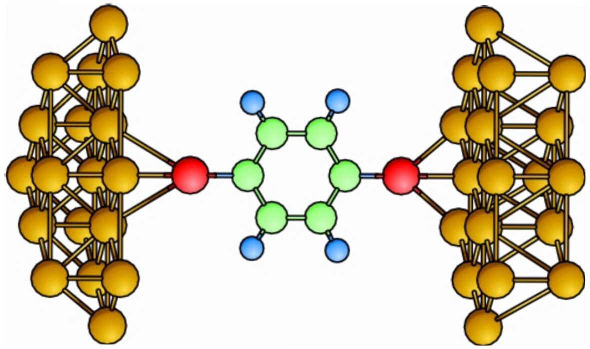
$$SS = m \times 2.3\, k_B T \;/\; q$$

S. Salahuddin and S. Datta, *Nano Letters*, Feb., 2008

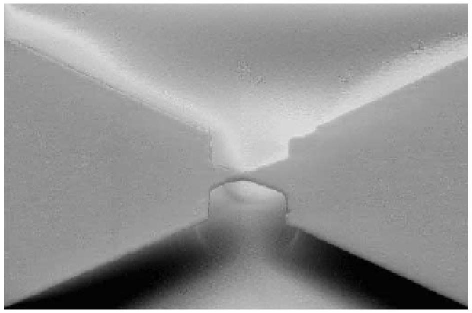
# outline

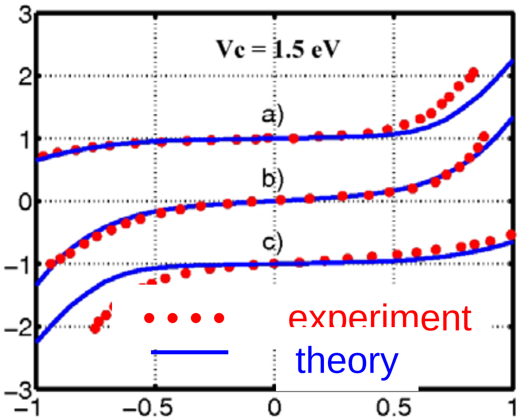
1) More Moore
2) ***More than Moore?***
3) 21st Century Computational Electronics
4) Conclusions

# molecular electronics



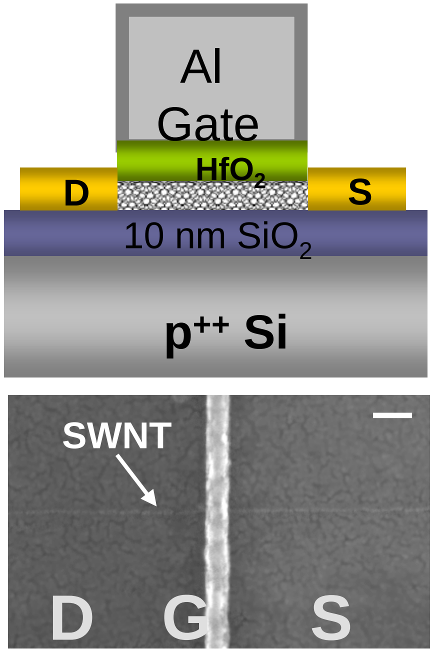
break junction



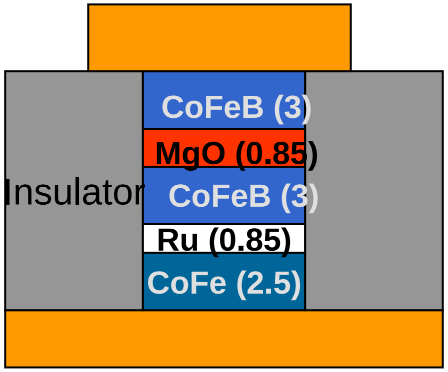


Weber group
*PRL*, **88**, 176804 (2002)

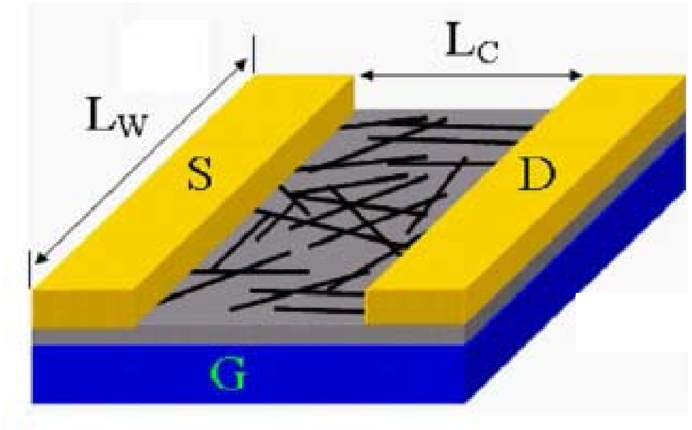
# new materials and devices



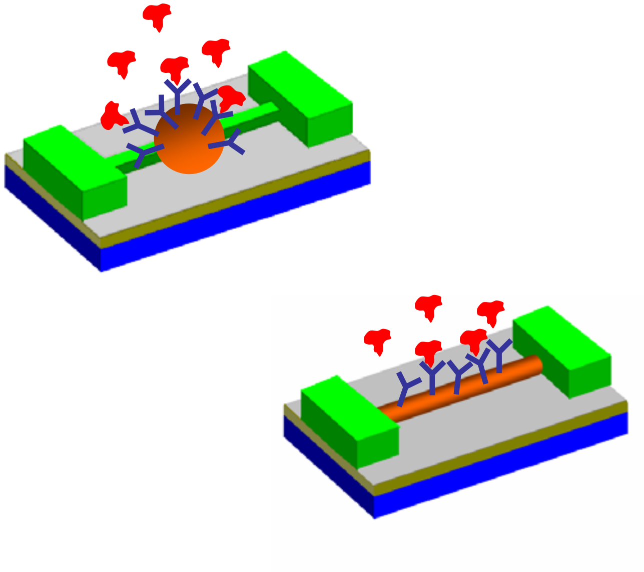
A. Javey, et al., *Nature*, **424**, 654, 2003.



Kubota et. al. , Jap. J. App. Phys., 2005



J. Rogers, et al.



# outline

1) More Moore
2) More than Moore?
3) **21st Century Computational Electronics**
4) Conclusions

# computational electronics

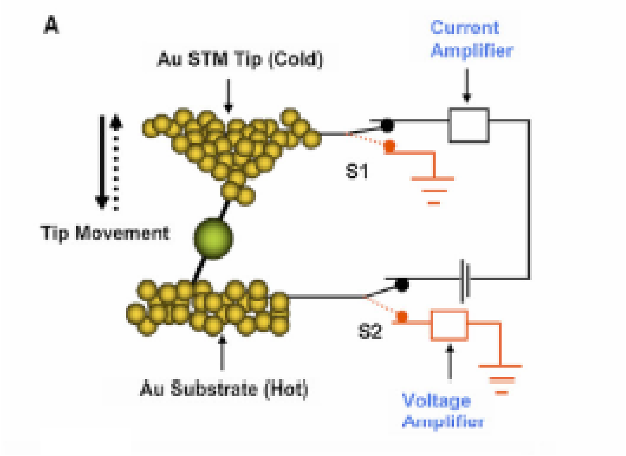
1) Increasing diversity of devices and materials (need for a unified approach)

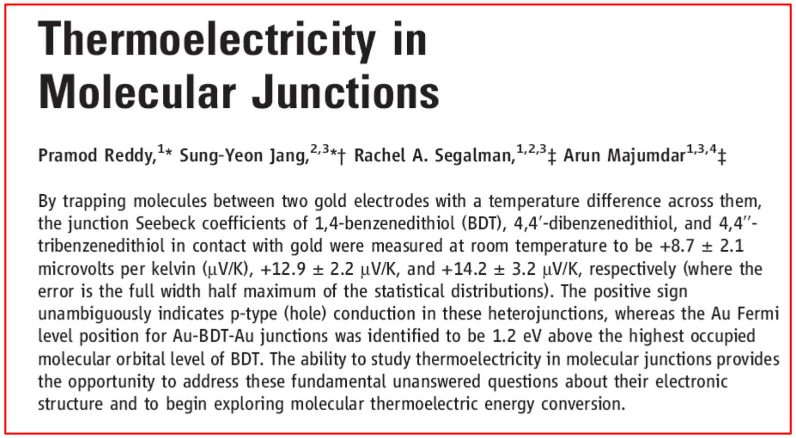
2) Increasing ‘difficulty’ of the problems

3) The future is still defining itself

4) Opportunities
    - -human health
    - -energy
    - -environment / climate
    - -security
    - -…

# Seebeck coefficient of a molecule

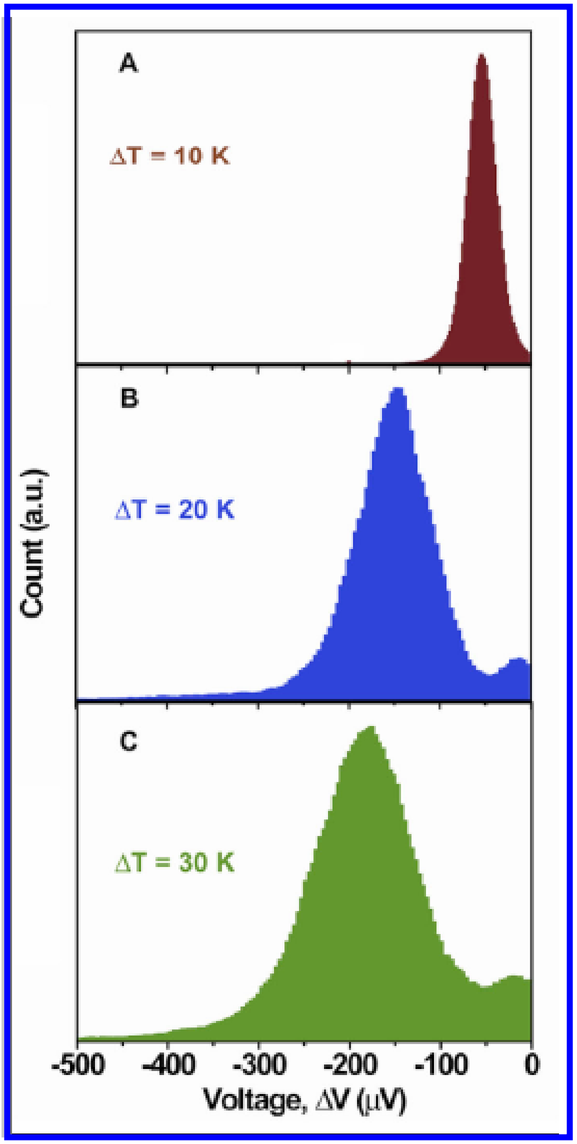




## Thermoelectricity in Molecular Junctions

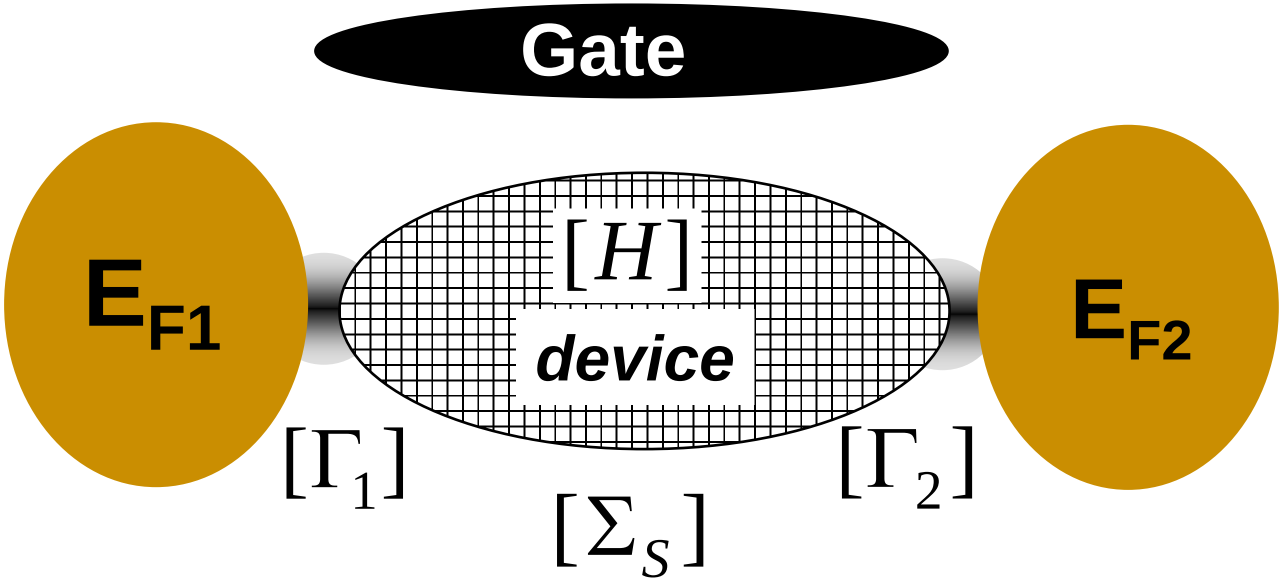
Pramod Reddy,[1]* Sung-Yeon Jang,[2,3]*† Rachel A. Segalman,[1,2,3]‡ Arun Majumdar[1,3,4]‡

By trapping molecules between two gold electrodes with a temperature difference across them, the junction Seebeck coefficients of 1,4-benzenedithiol (BDT), 4,4′-dibenzenedithiol, and 4,4′′-tribenzenedithiol in contact with gold were measured at room temperature to be +8.7 ± 2.1 microvolts per kelvin (μV/K), +12.9 ± 2.2 μV/K, and +14.2 ± 3.2 μV/K, respectively (where the error is the full width half maximum of the statistical distributions). The positive sign unambiguously indicates p-type (hole) conduction in these heterojunctions, whereas the Au Fermi level position for Au-BDT-Au junctions was identified to be 1.2 eV above the highest occupied molecular orbital level of BDT. The ability to study thermoelectricity in molecular junctions provides the opportunity to address these fundamental unanswered questions about their electronic structure and to begin exploring molecular thermoelectric energy conversion.



**Experiment:**
Reddy, et al., Science, **315** 16 March, 2005.
**Theory:**
Paulsson and Datta, PRB **67**, 241403 (2003),

# unified approach to nano-devices

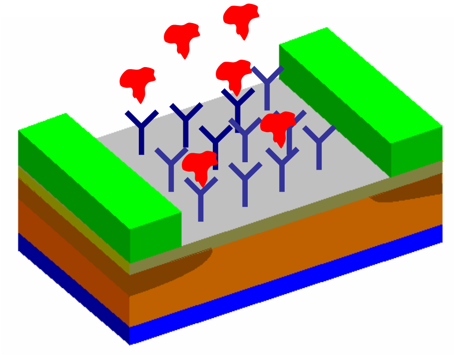


NEGF Approach to Quantum Transport

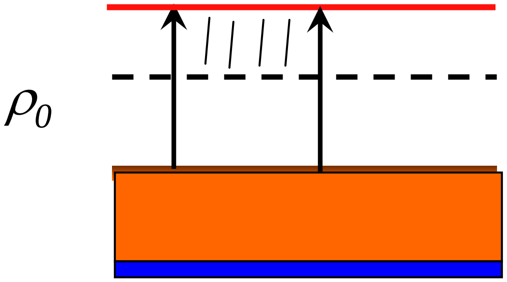
Supriyo Datta, “Concepts in Quantum Transport”

# solving the right problem

$D_F=2$



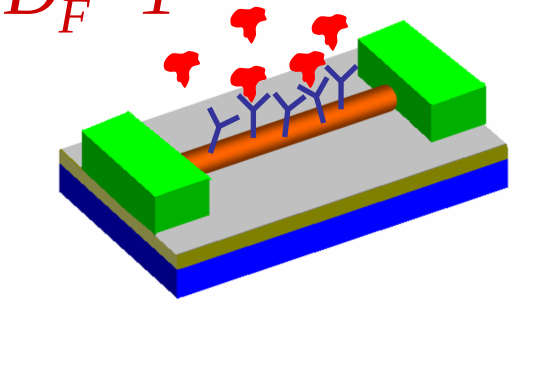
$R : \sqrt{Dt}$



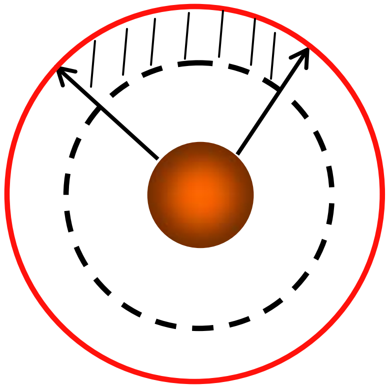
$$N(t) = \rho_0 \times R \times A$$

$$N(t) : \rho_0 \sqrt{Dt}$$

$D_F=1$



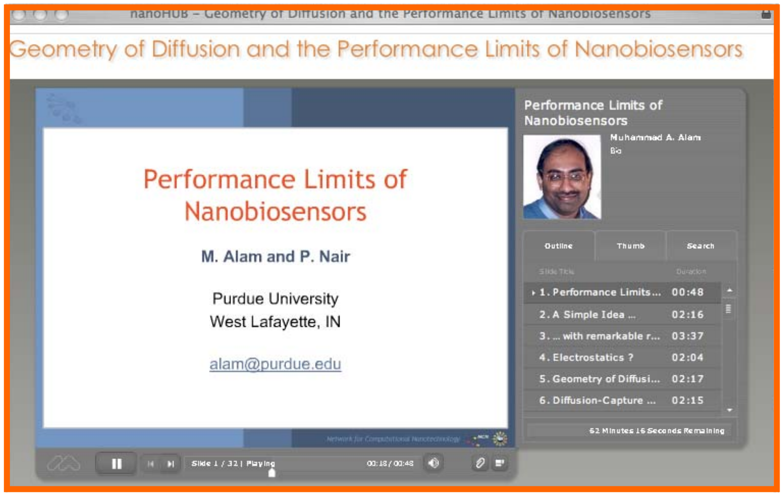
$R : \sqrt{Dt}$



$$N(t) = \rho_0 \times \pi R^2 \times L$$

$$N(t) : \rho_0 Dt$$

# bio-sensors (Alam)



nanoHUB – Geometry of Diffusion and the Performance Limits of Nanobiosensors

Geometry of Diffusion and the Performance Limits of Nanobiosensors

Performance Limits of Nanobiosensors

M. Alam and P. Nair

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Network for Computational Nanotechnology

Performance Limits of Nanobiosensors

Muhammad A. Alam
Bio

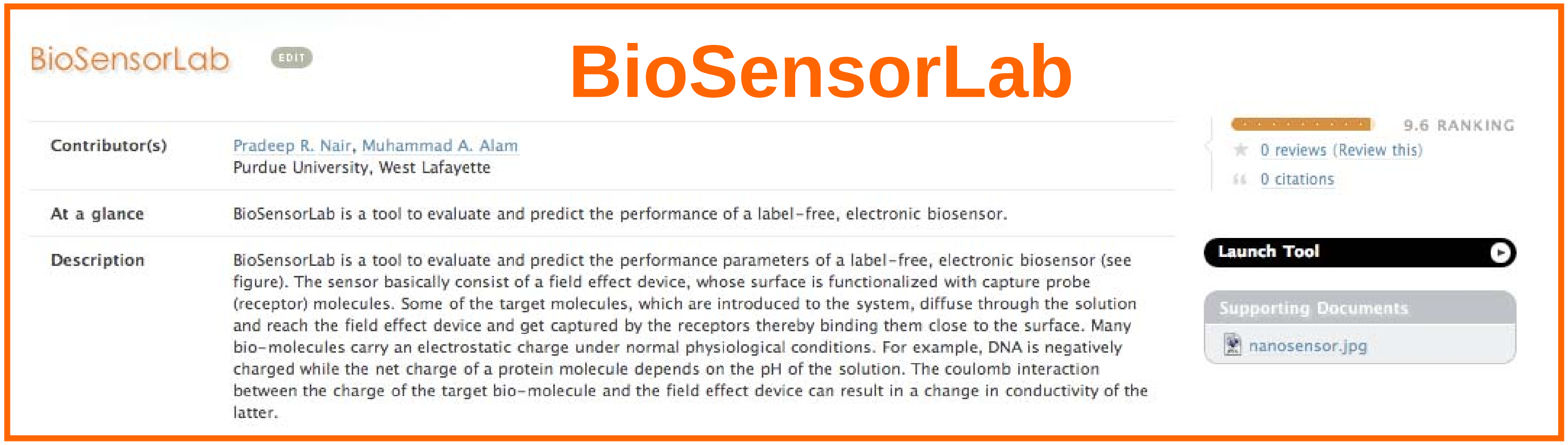
| Slide Title | Duration |
|---|---|
| 1. Performance Limits... | 00:48 |
| 2. A Simple Idea ... | 02:16 |
| 3. ... with remarkable r... | 03:37 |
| 4. Electrostatics ? | 02:04 |
| 5. Geometry of Diffusi... | 02:17 |
| 6. Diffusion-Capture ... | 02:15 |

62 Minutes 16 Seconds Remaining

Slide 1 / 32 | Playing 00:18 / 00:48

M.A. Alam, “Geometry of Diffusion and the Performance Limits of Nanobiosensors.”

## BioSensorLab



BioSensorLab

**Contributor(s)** Pradeep R. Nair, Muhammad A. Alam
Purdue University, West Lafayette

**At a glance** BioSensorLab is a tool to evaluate and predict the performance of a label-free, electronic biosensor.

**Description** BioSensorLab is a tool to evaluate and predict the performance parameters of a label-free, electronic biosensor (see figure). The sensor basically consist of a field effect device, whose surface is functionalized with capture probe (receptor) molecules. Some of the target molecules, which are introduced to the system, diffuse through the solution and reach the field effect device and get captured by the receptors thereby binding them close to the surface. Many bio-molecules carry an electrostatic charge under normal physiological conditions. For example, DNA is negatively charged while the net charge of a protein molecule depends on the pH of the solution. The coulomb interaction between the charge of the target bio-molecule and the field effect device can result in a change in conductivity of the latter.

9.6 RANKING
0 reviews (Review this)
0 citations

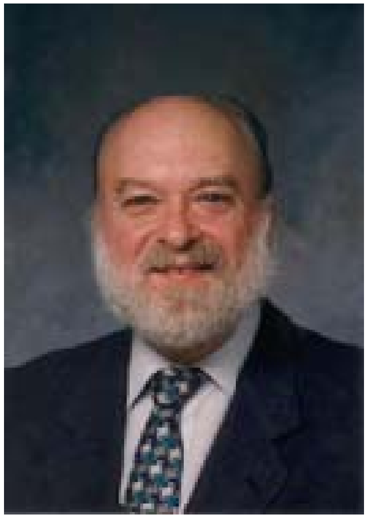
# excellence in computer simulation

"Excellent computer simulations are done for a purpose…

1) to **explore** uncharted territory

2) to **resolve** a well-posed scientific or technical question

3) to make a good **design** choice."



Leo P. Kadanoff

**"Excellence in Computer Simulation"**
**www.nanoHUB.org**

L.P. Kadanov, "Excellence in Computer Simulation,"
*Computing in Science and Engineering*, (Mar./Apr. 2004).
(see also, "Computational Scenarios," *Physics Today*, Nov. 2004).

# outline

1) More Moore
2) More than Moore?
3) 21st Century Computational Electronics
4) **Conclusions**

# shared research facilities

***Birck Nanotechnology Center, Purdue University***

Courtesy HDR Architecture, Inc./Steve Hall © Hedrich Blessing

# “service-oriented science”

Distributed Computing

VIEWPOINT

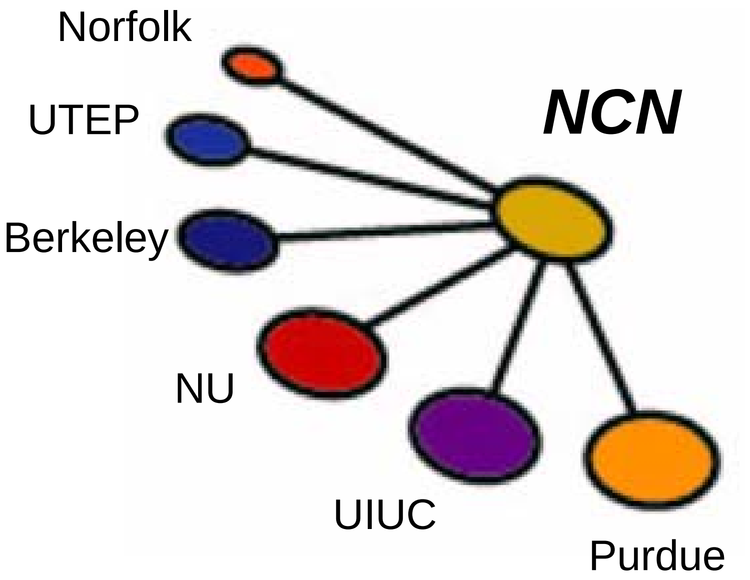
Service-Oriented Science

Ian Foster

New information architectures enable new approaches to publishing and Accessing valuable data and programs… as services….. Thus, **tools formerly accessible only to the specialist can be made available to all**;…Such service-oriented approaches to science are already being applied successfully, in some cases at substantial scales….

6 MAY 2005 VOL 308 SCIENCE www.sciencemag.org

# Network for Computational Nanotechnology

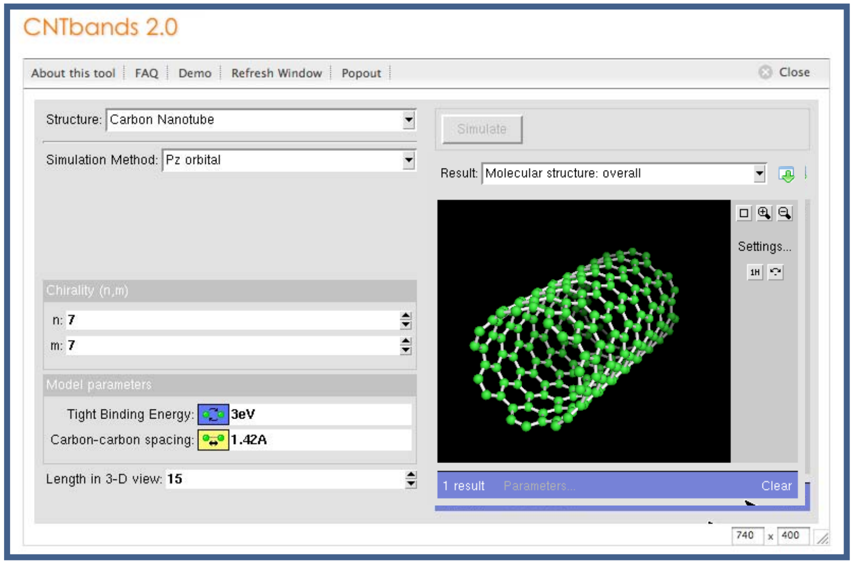


***cyberinfrastructure***

- connects computationalists and experimentalists
- bridges disciplines
- promotes collaboration
- supports computational science and engineering
- disseminates knowledge and services
- enables research and education

# online simulation

www.nanoHUB.org



Structure: Carbon Nanotube

Simulation Method: Pz orbital

Result: Molecular structure: overall

Chirality (n,m)

n: 7

m: 7

Model parameters

Tight Binding Energy: 3eV

Carbon-carbon spacing: 1.42A

Length in 3-D view: 15

740 x 400

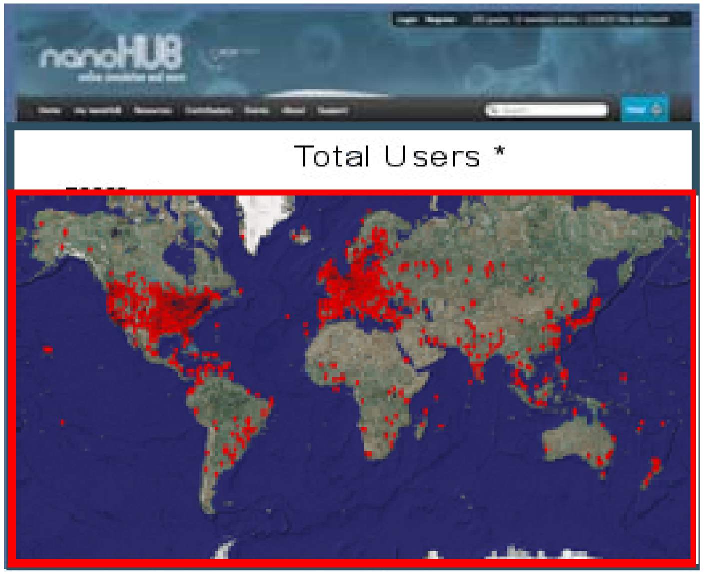
-**Rappture** for SW development
http://rappture.org

-**HUBzero** middleware for online simulation http:hubzero.org

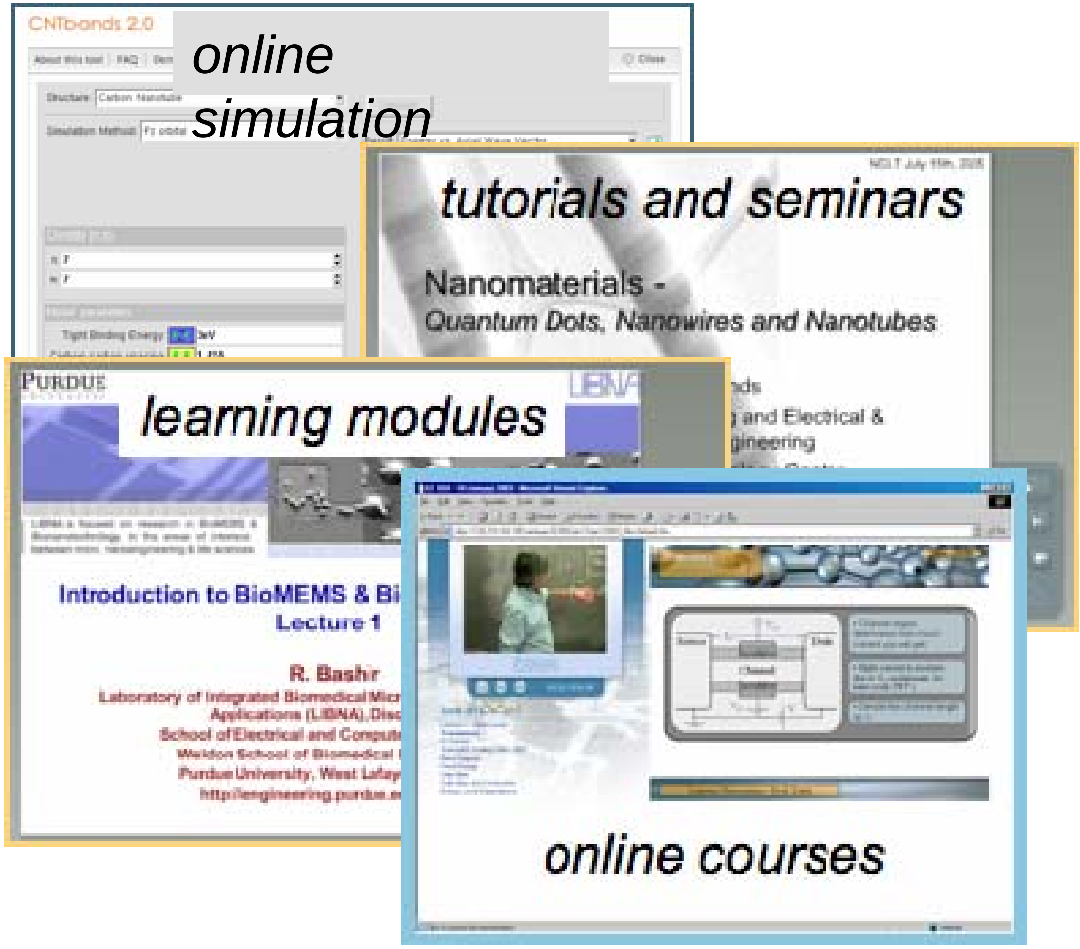
> 70 tools

# and more…..

NCN's science gateway



www.nanoHUB.org



+ *tools for collaboration*

# Summary

1) Device simulation must address a broader range of problems
2) Simulations must capture quantum and atomic scale effects
3) Computationalists and experimentalists must work together
4) Problem-solving and invention should be emphasized
5) Current tools must evolve and new tools may be necessary
6) Development of new codes must be accelerated

1999 Nanotransistor Meeting, NIST, Gathersberg, Md.

# Summary

1) There has never been a more interesting time for computational electronics.

2) We have an opportunity to help define a new field.

3) Cyberinfrastructure can help.