

CI Days 2010, Dec. 9, 2010

# nanoHUB.org:

## past, present, future...

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and

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# past

**PUNCH** Purdue University Network Computing Hubs  
Online Computing for Engineering and Science

Menu: Home, Getting started, About PUNCH, Policies, Statistics, System map, Credits, Sponsors, People, Contact us

Computational Electronics: Tools (Adept, FastHenry, Minimos, SDemon, Spice2G, UIFullBand, UIrode), Laboratories (Electromagnetics, Silicon)

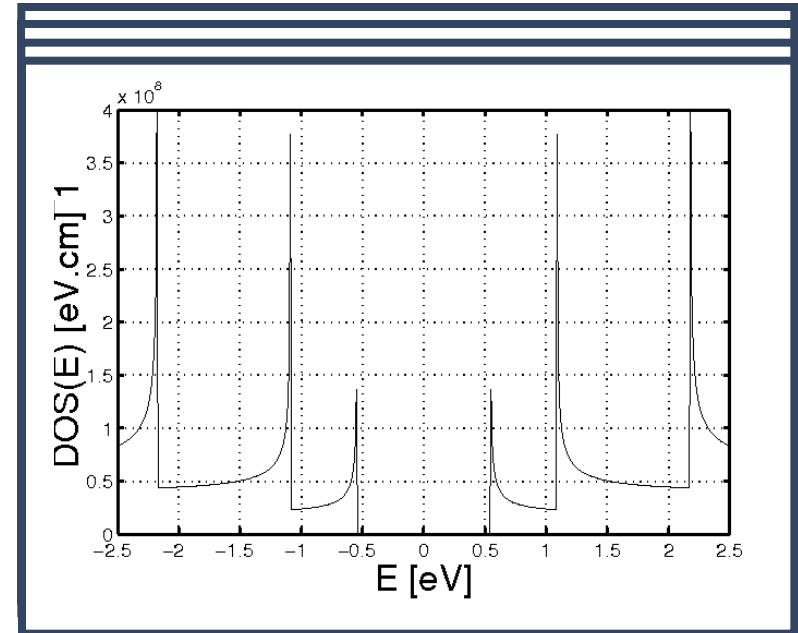
Computer Architecture: Login to use tools or Request free account. Tools (Demon, Fish-1D, Moca, SMASH, Suprem3, UTMariowe4.0)

Parallel Programming: Device, MOSCV, MolecularIV, Schred, TSuprem3, UTMinimos. Tool description: Calculates Density of States, Transmission Function, Resistance and Conductance Spectrum of molecular systems.

VLSI Design: FastCap, Medici, Prophet, Sequel

General / Productivity Tools: Ansys 5.5, Xfig 3.2, Matlab 5.3, Mentor Graphics, StarOffice

Demo Tools: GNU Chess



(with J. Fortes and N. Kapadia)

>7M hits (1994 - 2002)

1994  
●  
AT&T

2002  
●  
NCN

# Network for Computational Nanotechnology

*established in 2002:*

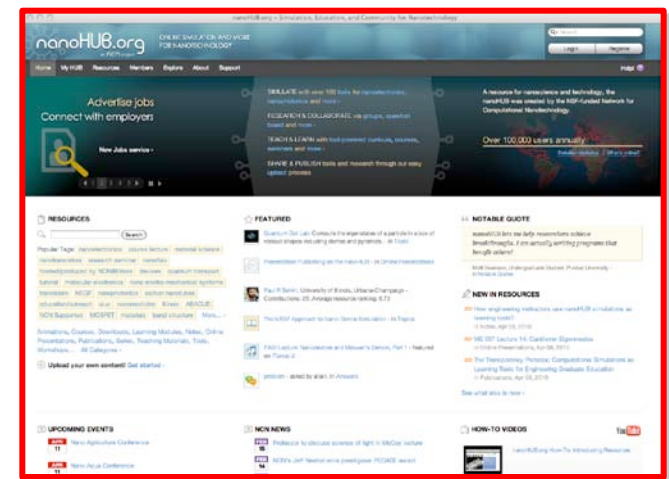
## **Mission:**

**Research** that helps move nanoscience to nanotechnology to nanomanufacturing.

## **Infrastructure to:**

- *connect experts in theory, modeling, and simulation to experimentalists*
- *promote cross-disciplinary and simulation-based education*
- *disseminate insights and understanding and research methods*

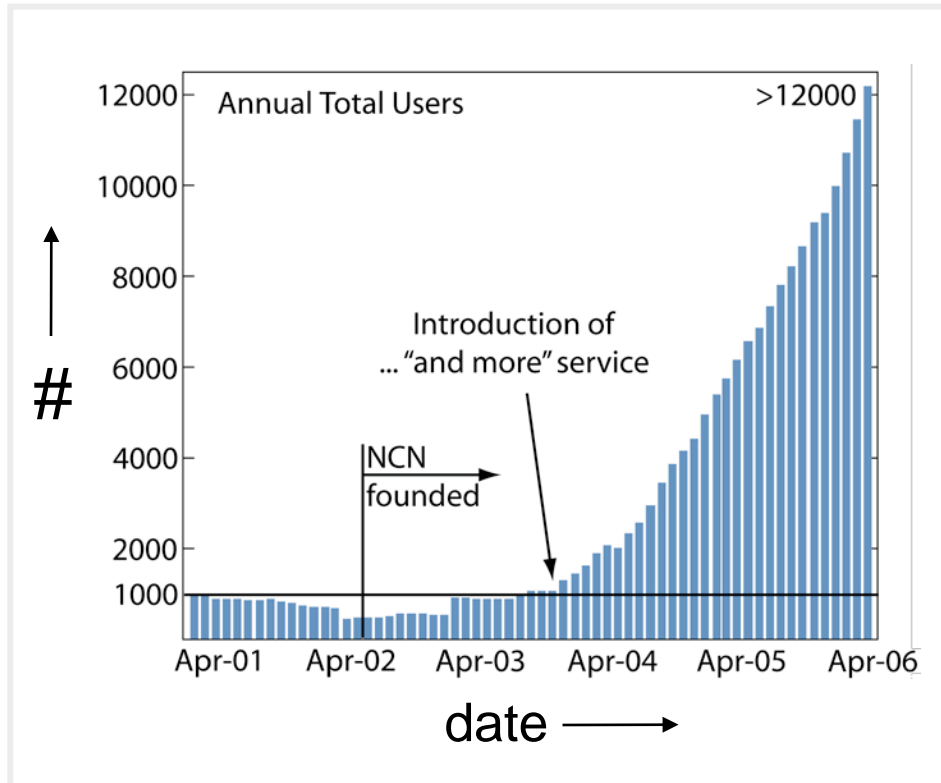
**Key strategy:**  
cyberinfrastructure



nanoHUB.org

- 1) “simulation at your fingertips”
- 2) online training
- 3) online learning
- 4) tools for collaboration

# online simulation and more



## on computing

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***“The purpose of computing is insight, not numbers.”***

R.W. Hamming (in the introduction to his book, *Introduction to Applied Numerical Analysis*, 1971.

“In this book Hamming taught that tailoring a numerical method to fit a physical problem, rather than blindly using a generic “all-purpose” routine, could provide insight into the problem by underlining its peculiarities.”

[http://en.wikipedia.org/wiki/Richard\\_Hamming](http://en.wikipedia.org/wiki/Richard_Hamming)

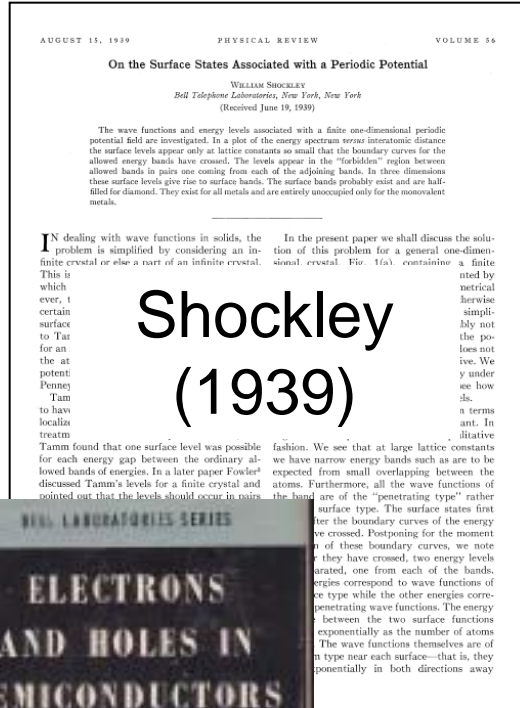


R.W. Hamming

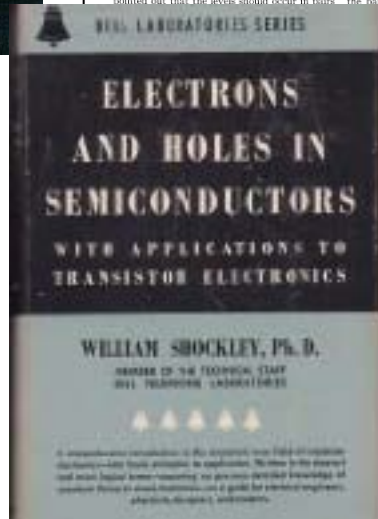
# the diffusion of knowledge



transistor (1948)



Shockley (1939)



Shockley (1951)

## Bell Labs Transistor Workshops (1950's)



**SEEC**

*R.B. Adler, et al., 1960-1967*

# Vlad Shalaev

ECE 696s Nanophotonics: 19,898 viewers

**Nanophotonics\***

Professor Vladimir M. Shalaev  
ECE695S

5  $\mu\text{m}$

**PhotonicRT: Wave Propagation in Multilayer Structures**

Tool Questions? About

1 Wave 2 Layers 3 Calculate

About this tool Questions?

This tool calculates the reflection (R), transmission (T) and absorption (A) of light passing through a lamellar structure with uniform isotropic layers. User defines the following parameters:

- Polarization of incident waves
- Incident angle of the waves
- Wavelength range
- Material in the front (source) side
- Multilayer structure (material and thickness for each layer)
- Material in the back (shade) side

FRONT

Layer 1 Layer 2 Layer 3 Layer 4 ... Layer N

BACK

Polarization: TE

Incident angle: 0deg

Layers >

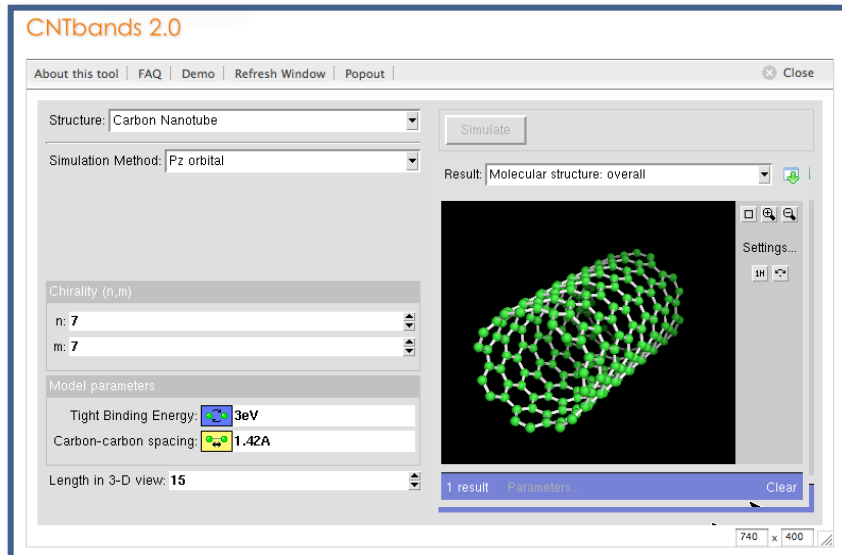
780 x 600



V.M. Shalaev  
Robert and Anne Burnett Professor  
2010 Max Born Award  
2010 Willis E. Lamb Award

# online simulation with Rappture

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More than 180  
simulation tools  
now online.

Rapid Application Infrastructure ([rappture.org](http://rappture.org))

Maxwell's Daemon middleware

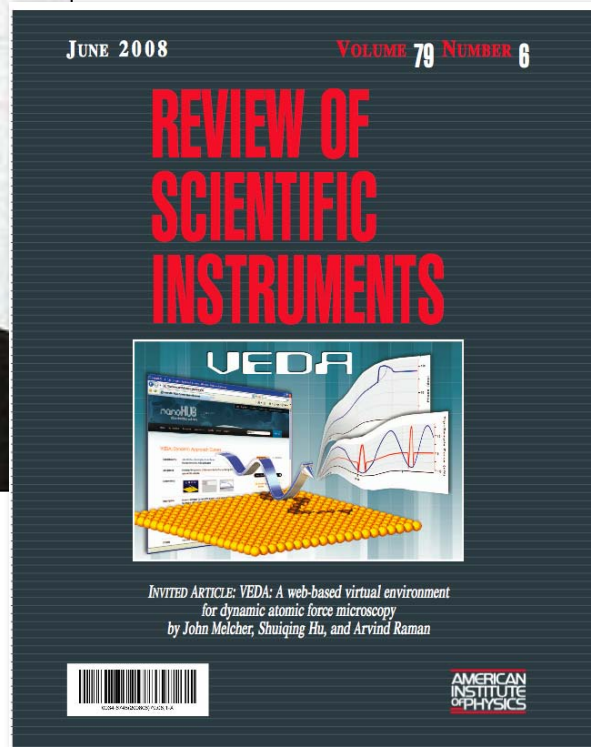
Nanoviz visualization



# Arvind Raman: Scanning Probe Microscopy



Arvind  
Raman



- In addition to scientists and students worldwide, VEDA is being used by all major US AFM companies such as Veeco, Agilent, and Asylum for both training and research.

ME 597/PHYS 570:  
***Fundamentals of Atomic Force Microscopy***

\* J. Melcher, S. Hu, A. Raman, “VEDA – a web based virtual environment for dynamic Atomic Force Microscopy”, *Invited article – Review of Scientific Instruments*, June 2008..



# NCN / nanoHUB.org

user community.....

students

professionals

faculty

HUBzero IT platform

user and site support, SW development, service development,  
content development, assessment...

research community.....

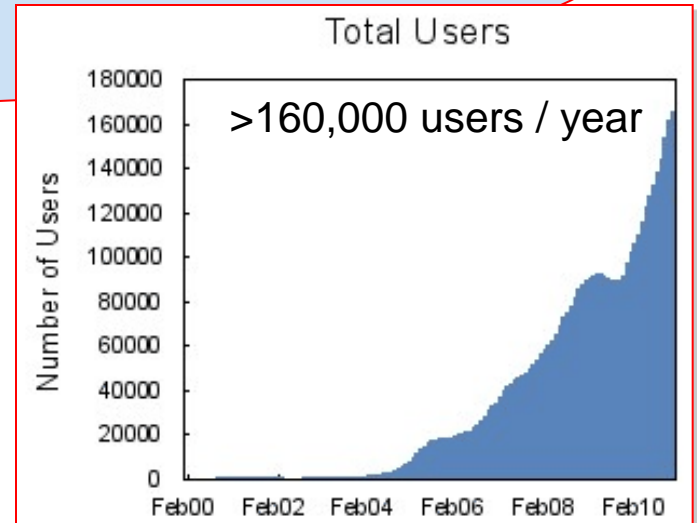
faculty

research groups

research centers

*technology for:*

- dissemination
- collaboration
- online simulation / data



# outcomes and directions

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- 1) nanoHUB is a demonstration of the effectiveness of cyberinfrastructure in collaboration, dissemination, and learning.
- 2) HUBzero is a unique (open-source) IT platform and the HUBzero community is a source of best practices and leveraged technology development.
- 3) Looking to the future, we continue to ask:
  - Outside: How can we better serve users?
  - Inside: How can we further engage faculty and graduate students?
  - \$\$: How do we sustain the effort?