

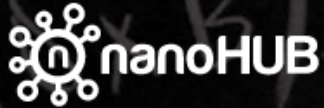
# Cloud simulations & data in nanoHUB: a tour & an invitation to collaborate



*Ale Strachan, Purdue University  
Deputy Director, nanoHUB  
[strachan@purdue.edu](mailto:strachan@purdue.edu)*

nanoHUB.org usage 2015-01-19 00:00:00

# nanoHUB



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# NANO is HUGE

LARGEST NANOTECHNOLOGY ONLINE RESOURCE

400

simulation tools

1.4M

visitors

4500

resources



National Science Foundation  
WHERE DISCOVERIES BEGIN



# much more than a web site



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# LEARN

EXPERT CLASSES AT YOUR OWN PACE

# much more than a web site



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# EXPLORE

THOUSANDS OF NANOTECHNOLOGY RESOURCES



# much more than a web site



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# SIMULATE

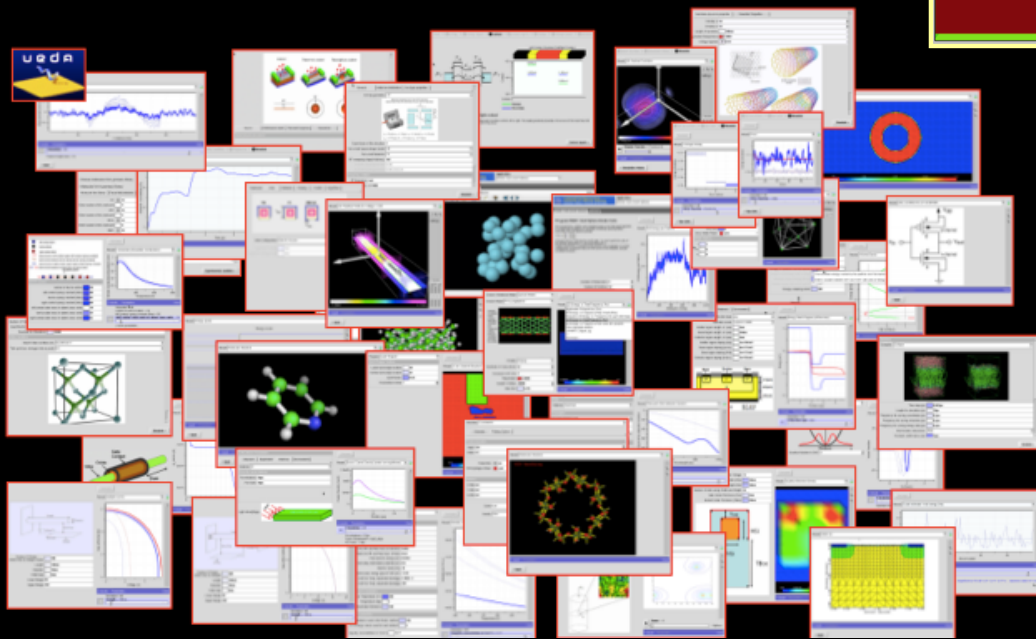
HUNDREDS OF CUTTING-EDGE TOOLS TO PROPEL YOUR RESEARCH

# nanoHUB

Making simulations & data universally accessible and useful

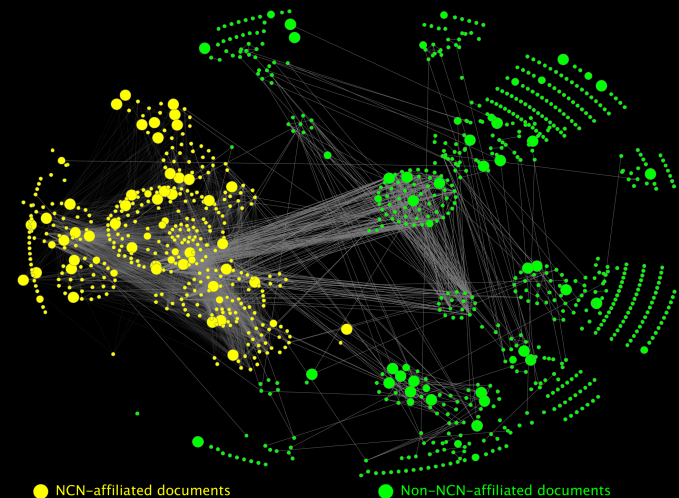
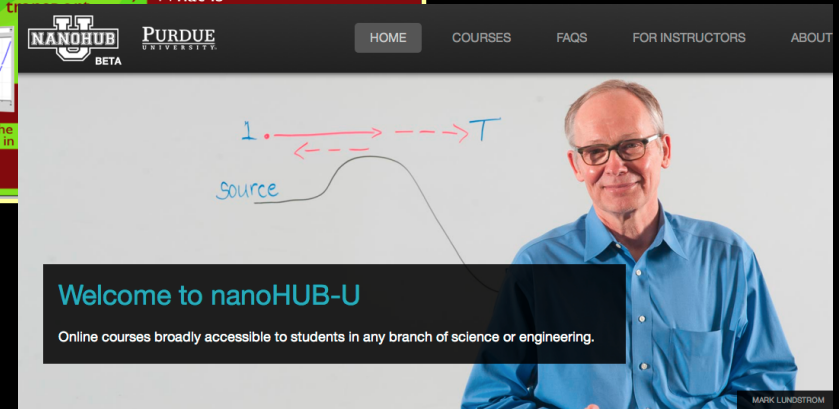
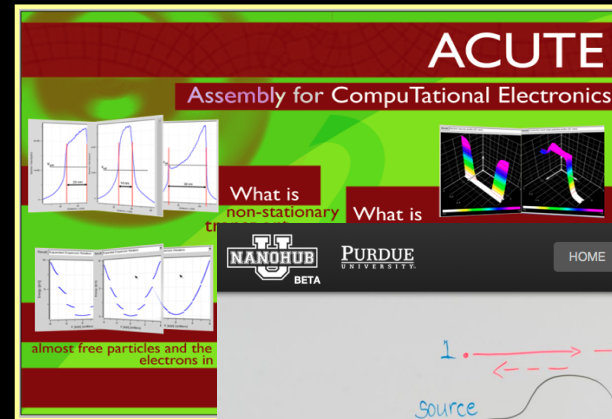
Research in the cloud

- 400+ simulation tools
- 2,500 online seminars



## Education

- nanoHUB-U
- 500+ teaching materials



● NCN-affiliated documents

● Non-NCN-affiliated documents

\* Small dots represent papers with relatively low secondary citations, medium dots indicate papers with potential to influence h-index, large dots represent papers affecting the h-index





# nanoHUB



- Community driven



1,600+ contributors

- NCN-cyber node develops & operates the cyberinfrastructure



- Making simulations and data universally accessible & useful
  - Towards decision-making and knowledge



# Tools designed for end users

Nanomaterial mechanics explorer

1 Input → 2 Simulate

Mechanics Lab

Experiment: Nanowire

Nanowire

Nanowire Material and Orientation: Nickel [100]

**Crack Propagation**

**Phase Transition**

**Nanowire Tensile Test**

**Dislocation Dynamics**

**Nanowire Tensile Test Default Settings**

Simulate >

DFT Material Properties Simulator

1 Input → 2 Simulate

Basic Input

Task: E-K Diagrams

Material Type: Semiconductor

Semiconductors: Si

Advanced Options:  no

Simulate >

Storage (manage) 56% of 20GB

850 x 650

3:15 PM – 5:00 PM Hands-on Materials Data Demos/Exhibits & Kickoff Reception  
(Norris–Louis Room)  
Exhibitors: ASM, Citrine, MagPie, Materials Data Facility,  
Materials Resource Registry, Materials Data Curator System, National Data  
Services, NanoHub, NanoMine, NIMS MatNavi, NoMaD, OQDB





# Impact on research

nanoHUB Citation Network (2000–2016)

1,714 papers

4,049+ authors

258 authors from industry

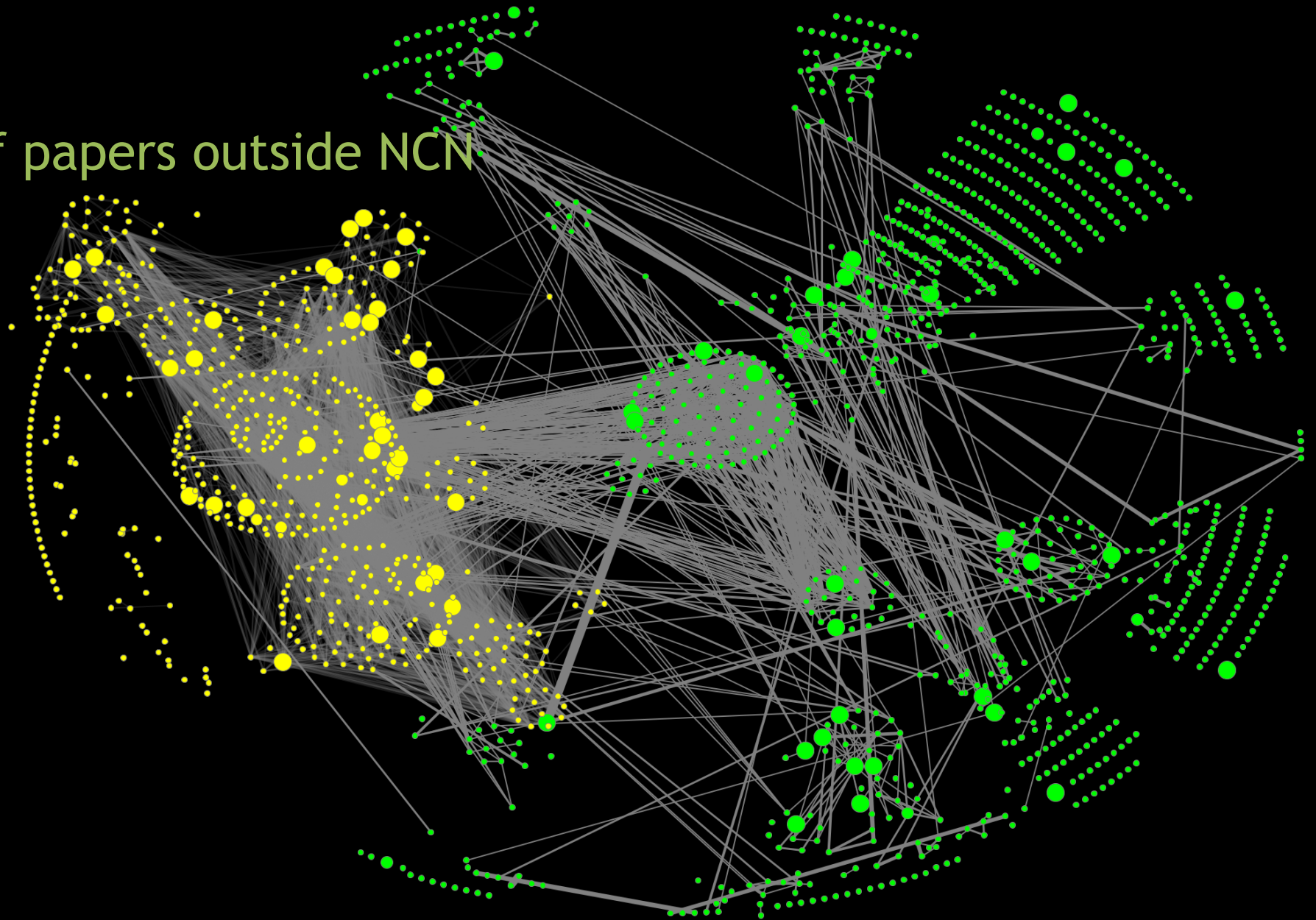


- Three distinct dot sizes indicate the level of influence on h-index
- Papers with relatively low secondary citations
- Papers with potential to influence h-index
- Papers affecting the h-index



# NCN vs. Non-NCN (2000–2016)

64% of papers outside NCN



● NCN-affiliated documents

● Non-NCN-affiliated documents

- Three distinct dot sizes indicate the level of influence on h-index
- Papers with relatively low secondary citations
- Papers with potential to influence h-index
- Papers affecting the h-index



# nanoHUB is a publisher

OPTICS LETTERS / Vol. 36, No. 8 / April 15, 2011

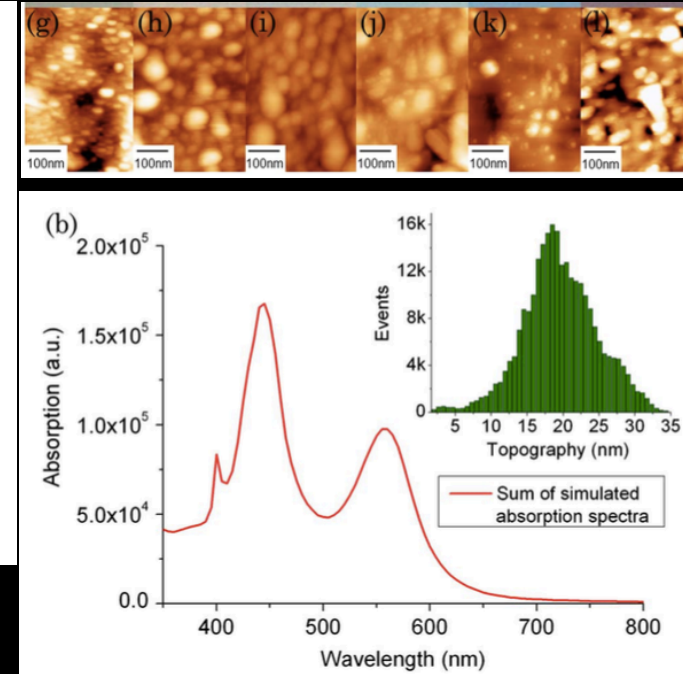
## Engineering the plasmon resonance of large area bimetallic nanoparticle films by laser nanostructuring for chemical sensors

Michail J. Beliatis, Simon J. Henley,\* and S. Ravi P. Silva

Nano-Electronics Centre, Advanced Technology Institute, University of Surrey, Guildford, GU2 7XH, UK

\*Corresponding author: s.henley@surrey.ac.uk

Received July 23, 2010; revised March 2, 2011; accepted March 15, 2011;  
posted March 23, 2011 (Doc. ID 132119); published April 7, 2011



## Extinction, Scattering and Absorption efficiencies of multilayer nanoparticles

By Bala Krishna Juluri, Jun Huang, Lasse Jensen

Pennsylvania State University

Calculates the extinction, scattering, and absorption efficiencies of single nanoparticle (1 layer), core-shell Nanoparticle (2 layer) and nanomatrix nanoparticle (3 layer)

| Version                | Released    | DOI Handle  |
|------------------------|-------------|---|
| <a href="#">1.03UQ</a> | 03 May 2016 | <a href="https://doi.org/10.4231/D3TH8BP1C">doi:10.4231/D3TH8BP1C</a> |
| <a href="#">1.03</a>   | 04 Aug 2014 | <a href="https://doi.org/10.4231/D37W6765J">doi:10.4231/D37W6765J</a> |
| <a href="#">1.02</a>   | 19 Oct 2012 | <a href="https://doi.org/10.4231/D3DB7VP65">doi:10.4231/D3DB7VP65</a> |
| <a href="#">1.01</a>   | 29 Apr 2010 | <a href="https://doi.org/10.4231/D3PV6B66Z">doi:10.4231/D3PV6B66Z</a> |
| <a href="#">1.0</a>    | 29 Jan 2010 | <a href="https://doi.org/10.4231/D3VX0631H">doi:10.4231/D3VX0631H</a> |

Sponsored by Penn State Center for Nanoscale Science (MRSEC)



# nanoHUB tools indexed by Web of Science

WEB OF SCIENCE™

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(from All Databases)

You searched for: PUBLICATION  
NAME: (nanoHUB) ...More

**Refine Results**

Search within results for...

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**Research Domains**

SCIENCE TECHNOLOGY (2,251)

Refine

**Research Areas**

SCIENCE TECHNOLOGY OTHER TOPICS (2,251)



Refine

**Document Types**

**Authors**

**Authors - Korean**

Sort by: Relevance

Select Page |   | Save to EndNote online | Add to Marked List

1. **NanoTCAD VIDES**  
By: Fiori, Gianluca; Iannaccone, Giuseppe  
nanoHUB  
DOI: <http://dx.doi.org.ezproxy.lib.purdue.edu/10.4231/D3RJ48T8X> Version: version 1.21  
Document Type: Software  
[View Abstract](#)
2. **Piece-Wise Constant Potential Barriers Tool**  
By: Wang, Xufeng; Agarwal, Samarth; Klimeck, Gerhard; et al.  
nanoHUB  
DOI: <http://dx.doi.org.ezproxy.lib.purdue.edu/10.4231/D3R20RX39> Version: version 1.2.8  
Document Type: Software  
[View Abstract](#)
3. **[Illinois]: Sigmoidal unit training with the delta rule**  
By: Sproat, Lisa  
nanoHUB  
DOI: <http://dx.doi.org.ezproxy.lib.purdue.edu/10.4231/D3S756K2N> Version: version 1.0a  
Document Type: Software  
[View Abstract](#)
4. **Adept**  
By: Anonymous  
nanoHUB  
DOI: <http://dx.doi.org.ezproxy.lib.purdue.edu/10.4231/d35q4rk5k> Version: version 1.0  
Document Type: Software  
[View Abstract](#)





# Re-thinking simulations

Thermoelectric Power Factor Calculator for Superlattices

Basic Model Configuration | Advanced Model Configuration

Temperature:

Temperature Gradient:

Si doping:

Ge doping:

Substrate composition Si(x)Ge(1-x):

Mat 1 Material:

Mat 2 Material:

Mat 1 Horizontal Thickness:

Mat 2 Horizontal Thickness:

Thermal Gradient

Simulate

Result: Seebeck Coefficient

| Mat 2 Horizontal Thickness (nm) | Seebeck Coefficient (uV/K) |
|---------------------------------|----------------------------|
| 1                               | ~200                       |
| 1.2                             | ~250                       |
| 1.5                             | ~300                       |
| 1.8                             | ~350                       |
| 2                               | ~450                       |
| 2.5                             | ~1100                      |
| 3                               | ~1700                      |

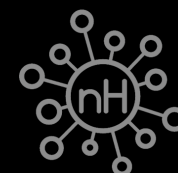
7 results Clear One Clear All

Simulation = #7

All ▶ Mat 2 Horizontal Thickness = 3nm

Storage (manage) 47% of 20GB

780 x 600



# Simulation tools are limited by infrastructure

The screenshot displays the 'Thermoelectric Power Factor Calculator' software interface. The window title is 'Thermoelectric Power Factor Calculator - Superlattice'. The interface is divided into several sections:

- Basic Model Configuration:** Includes a 'Simulate' button and an 'About this tool' link.
- Simulation Parameters:**
  - Temperature: 300 K
  - Temperature Gradient: 1 K
  - SI doping:  $1e+18 / \text{cm}^3$
  - Ge doping:  $1e+18 / \text{cm}^3$
  - Substrate composition:  $(x)\text{Ge}(1-x)$  with a value of 1
  - Mat 1 Material: Silicon
  - Mat 2 Material: Germanium
  - Mat 1 Horizontal Thickness: 1nm
- Simulation Instructions:** A text box stating 'Press Simulate to view results.'
- Device Schematic:** A diagram showing a cross-section of a device. It consists of a central 'Mat 2' layer (blue) flanked by 'Mat 1' layers (green), which are further flanked by 'Substrate' layers (purple). Arrows indicate the thickness of each layer. A 'Thermal Gradient' arrow points from left to right across the device.

The bottom of the screenshot shows a Windows taskbar with the following information: Storage (manage), 47% of 20GB, a refresh icon, a circular icon, and system tray icons for network (78%) and volume (60%).





# Simulation tools are limited by infrastructure



- Automatic uncertainty quantification in ALL nanoHUB tools
- New ways of executing tools - connecting tools with data exploration
- Connecting nanoHUB to other cyber-resources



# Your tool ... more powerful in nanoHUB

Thermoelectric Power Factor Calculator for Superlattices

Settings Terminate Keep for later

Basic Model Configuration | Advanced Model Configuration

Simulate new input parameters About this tool Questions?

Temperature: 300K

Temperature Gradient: 10K

Si doping:  $1e+18/cm^3$

Ge doping: gaussian  $1e+18/cm^3$

Substrate composition Si(x)Ge(1-x): 1

Mat 1 Material: Silicon

Mat 2 Material: Germanium

Mat 1 Horizontal Thickness: uniform 0.9nm 1.1nm

Mat 2 Horizontal Thickness: gaussian 1nm 0.08nm

Result:

Substrate Mat 1 Mat 2 Mat 1 Substrate

Mat 1 Thickness Mat 2 Thickness

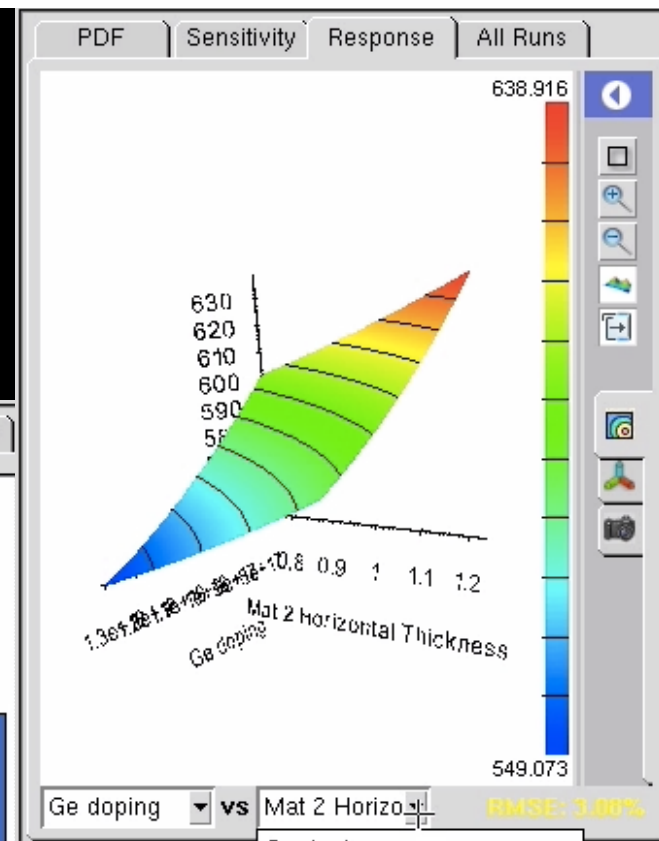
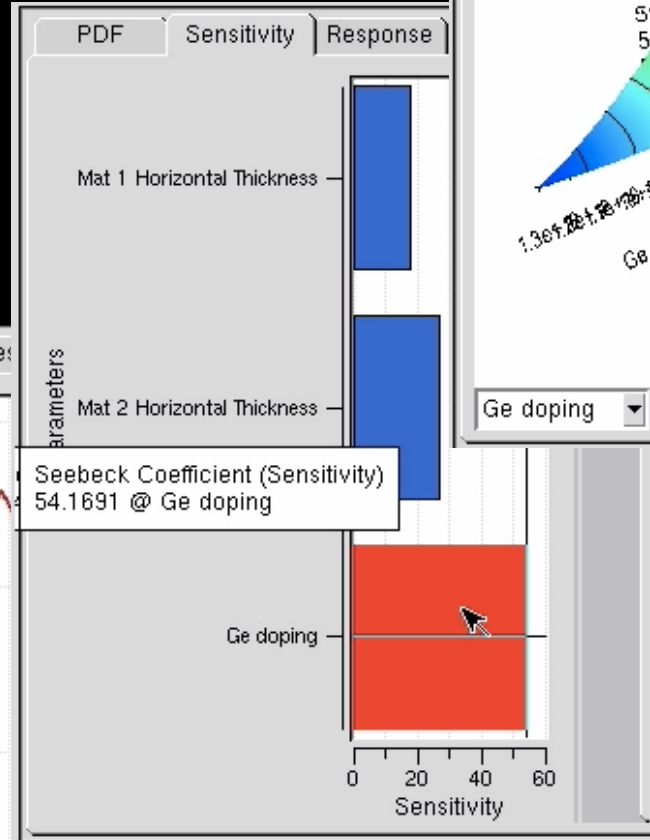
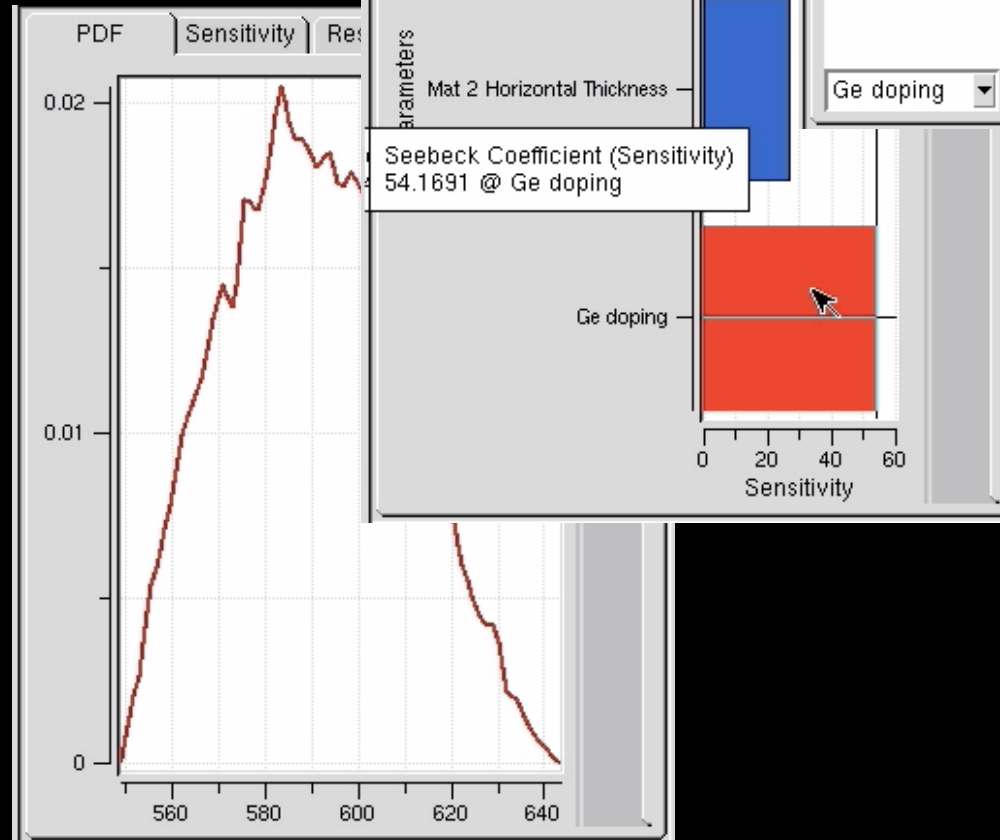
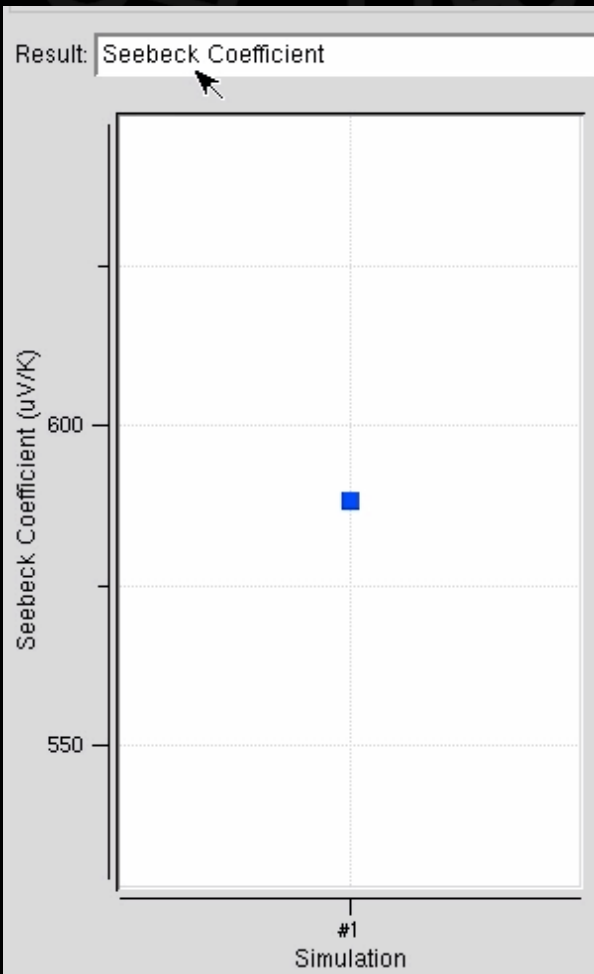
No results Clear

Storage (manage) 85% of 20GB 780 x 600

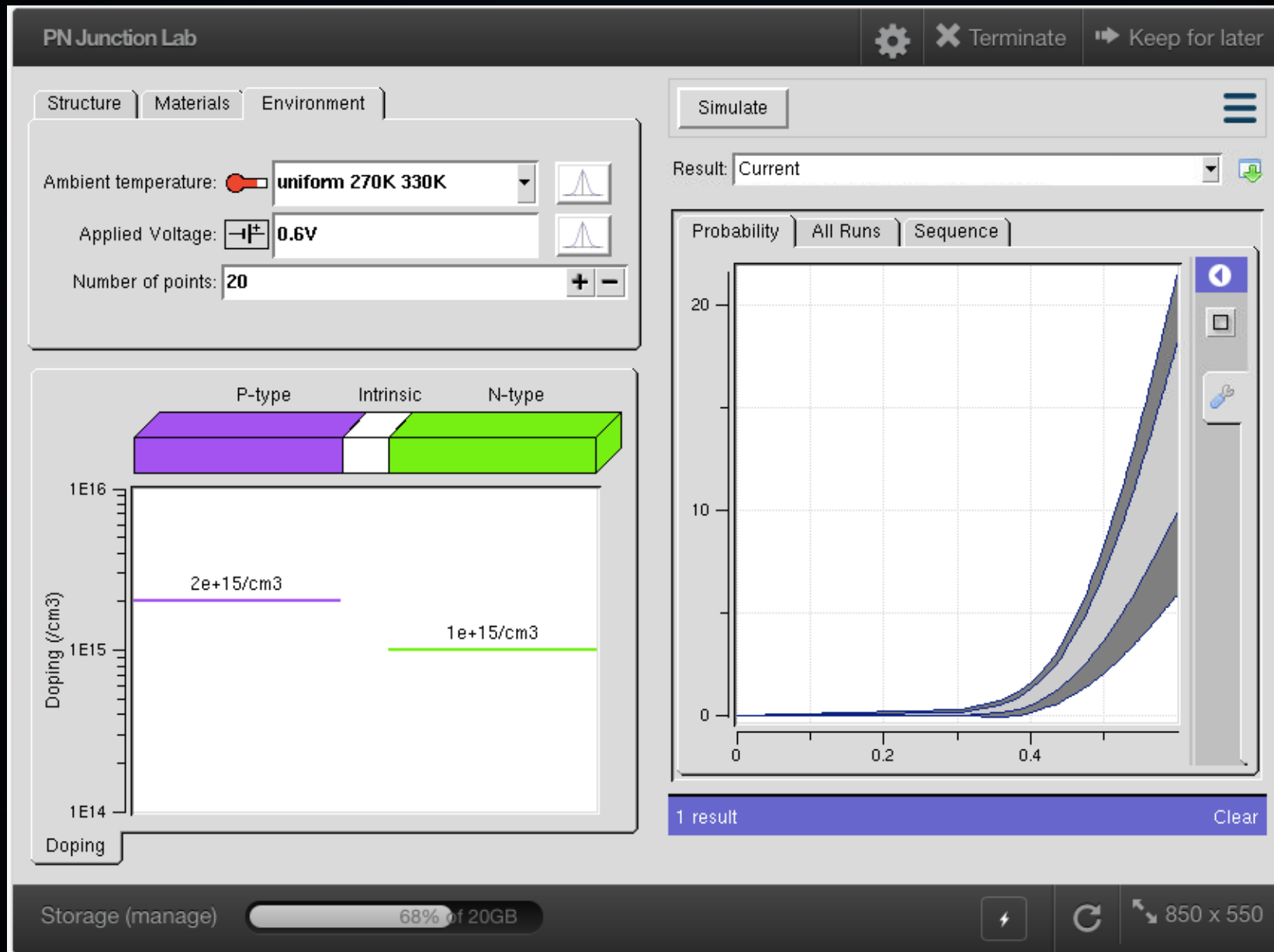




# Automatic UQ in nanoHUB



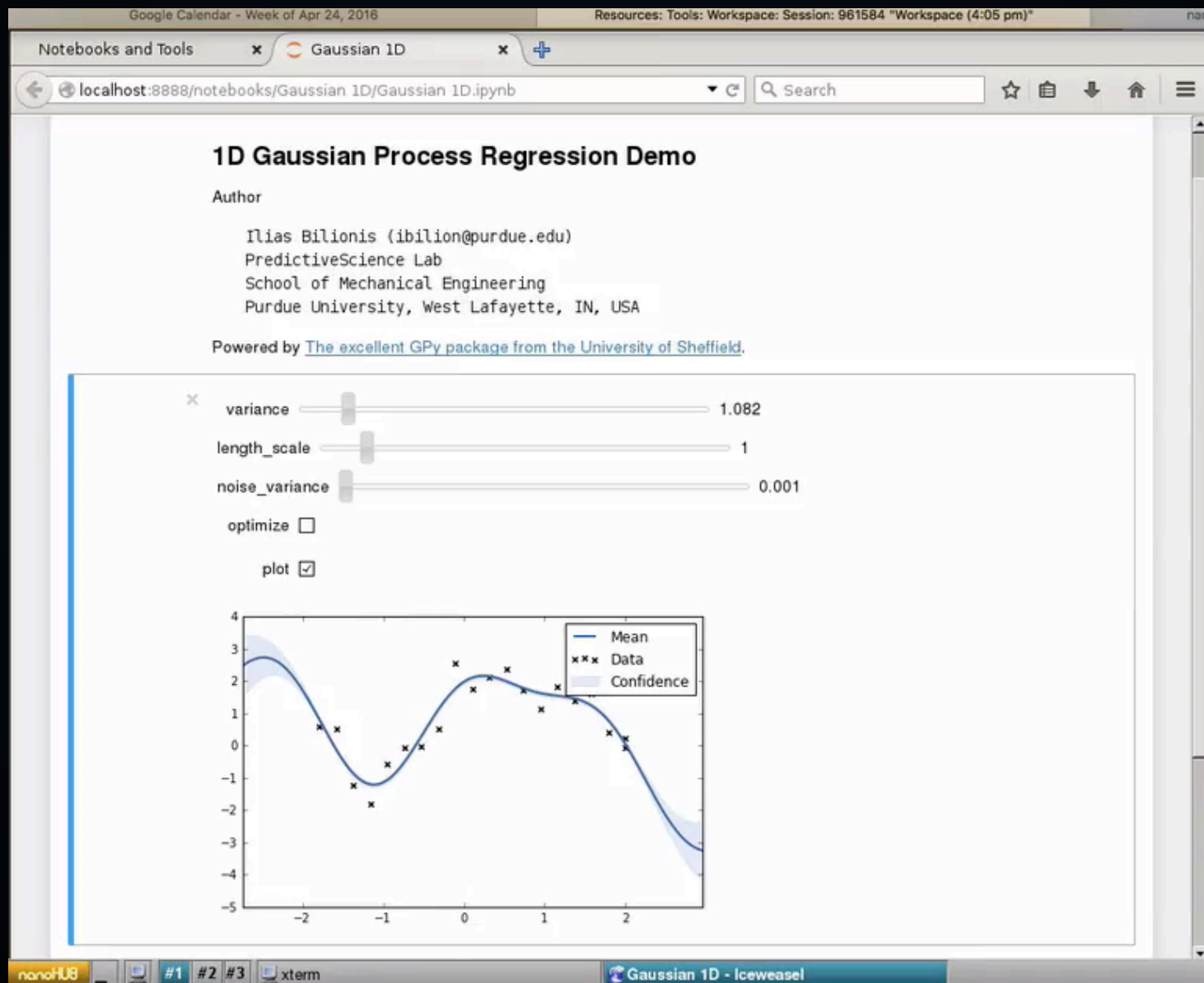
# Rigorous error bars in 1D curves





# Modern interface, instant feedback

## nanoHUB python notebooks



# nanoHUB -KIM collaboration



Knowledge of Interatomic Models  
NSF Cyberenabled Discovery & Innovation  
Ellad Tadmor, Ryan Elliot, J. Sethna

## KIM Models

Click on an element in the periodic table for which you need an interatomic model.

KIM Models (interatomic potentials and force fields) are software packages for describing atomic interactions that can be used with a variety of simulation codes, including LAMMPS, DL\_POLY, IMD, ASE and GULP, that are compatible with the KIM API standard.

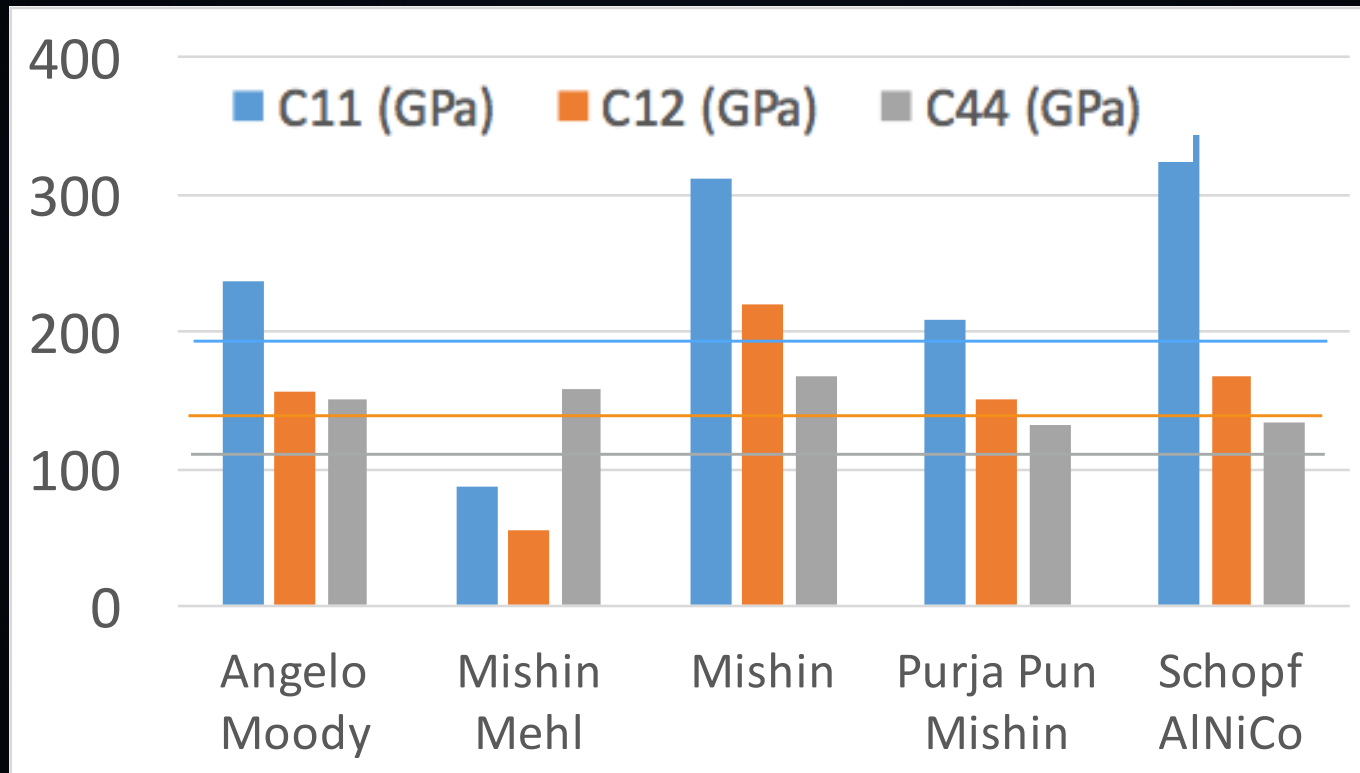
|    |    |    |    |    |    |    |    |    |    |    |    |     |    |     |    |     |     |
|----|----|----|----|----|----|----|----|----|----|----|----|-----|----|-----|----|-----|-----|
| H  |    |    |    |    |    |    |    |    |    |    |    |     |    |     |    |     | He  |
| Li | Be |    |    |    |    |    |    |    |    |    |    | B   | C  | N   | O  | F   | Ne  |
| Na | Mg |    |    |    |    |    |    |    |    |    |    | Al  | Si | P   | S  | Cl  | Ar  |
| K  | Ca | Sc | Ti | V  | Cr | Mn | Fe | Co | Ni | Cu | Zn | Ga  | Ge | As  | Se | Br  | Kr  |
| Rb | Sr | Y  | Zr | Nb | Mo | Tc | Ru | Rh | Pd | Ag | Cd | In  | Sn | Sb  | Te | I   | Xe  |
| Cs | Ba |    | Hf | Ta | W  | Re | Os | Ir | Pt | Au | Hg | Tl  | Pb | Bi  | Po | At  | Rn  |
| Fr | Ra |    | Rf | Db | Sg | Bh | Hs | Mt | Ds | Rg | Cn | Uut | Fl | Uup | Lv | Uus | Uuo |

# nanoHUB tool connecting to KIM

The screenshot shows the OpenKIM Explorer interface within a nanoHUB workspace. The browser address bar indicates the workspace session ID: 961584. The page title is "OpenKIM Explorer" and the session ID is 962237. The interface includes a "Query" section with a dropdown for "KIM object type" set to "Models" and a text input for "Elements" with the placeholder "Enter element symbols here". Below this is a checkbox for "Run LAMMPS with results of query" which is currently set to "no". A "Simulate" button is highlighted in yellow, with a tooltip that says "new input parameters". The main content area is titled "OpenKIM Explorer" and contains the text "Explore the OpenKIM repository and use it to drive LAMMPS". The bottom status bar shows "Storage (manage)" at 68% of 20GB, a refresh icon, and a resolution of 780 x 600.



# Make a decision about your research



# IDENT: sparse data exploration tool

& Navigation Tool

Interactive Data Exploration

for Nano Technology

The screenshot displays the IDENT software interface. At the top, there is a dropdown menu currently set to "Nothing selected", with "Use columns" and "Custom column" buttons to its right. Below this is a search input field containing the word "Search". A dropdown menu is open, listing various data exploration options. The options are: "Absorbance:as a function of Solvent", "Absorbance:as a function of Time", "pH", "Size:as a function of Light Exposure", "Size:as a function of Temperature", "Surface Area", "Bulk Density (g/cm^3)", "Specific Surface Area", "Surface Charge", "Electrophoretic Mobility", and "Zeta Potential (mV)". The background of the interface shows a grid of data points.

Nanomaterials registry: <https://nanohub.org/resources/22014>



# Select the area of interest

Nothing selected Use columns Custom column

288 total rows Edit filters

| ID | Mean Diameter (nm) | Mean Hydrodynamic Diameter (nm) | DisplayName |   |
|----|--------------------|---------------------------------|-------------|---|
| 6  |                    |                                 | Ag          | ⬇ |
| 7  | 7.2                |                                 | Ag NP       |   |
| 8  | 20.8               | 32                              | Ag NP       |   |
| 9  | 29                 | 39.6                            | Ag NP       |   |
| 10 | 43.4               | 47.6                            | Ag NP       |   |
| 11 | 41.9               | 43.1                            | Ag NP       |   |
| 12 | 49.1               | 59.2                            | Ag NP       |   |
| 13 | 53.5               | 57.1                            | Ag NP       |   |
| 14 | 57.7               | 68.3                            | Ag NP       |   |
| 15 | 8.2                |                                 | Ag NP       |   |
| 16 | 19.2               |                                 | Ag NP       | 🔒 |

Nanomaterials Registry Dataset

**Data of interest**

**Visualize your data**

Add a visualization +





# Visualize your data




# IDENT: Data Exploration & Tool Execution

Nothing selected Use columns Custom column 201 total rows

| ID  | Tool | Substrate x        | Substrate y        |
|-----|------|--------------------|--------------------|
| 95  |      | 0.05               | 1                  |
| 97  |      | 0.05               | 0.05               |
| 98  |      | 0.05               | 0.05               |
| 99  |      | 0.05               | 0.05               |
| 100 |      | 0.05               | 0.05               |
| 201 |      | 0.1                | 0.1                |
| 59  |      | 0.5225549349546599 | 0.5971173172672908 |
| 37  |      | 0.5228235114566167 | 0.709023382016227  |
| 41  |      | 0.5272180750363196 | 0.7838170306444151 |

III-V Strain Compensation Calculator

density estimate



# IDENT: Data Exploration & Tool Execution

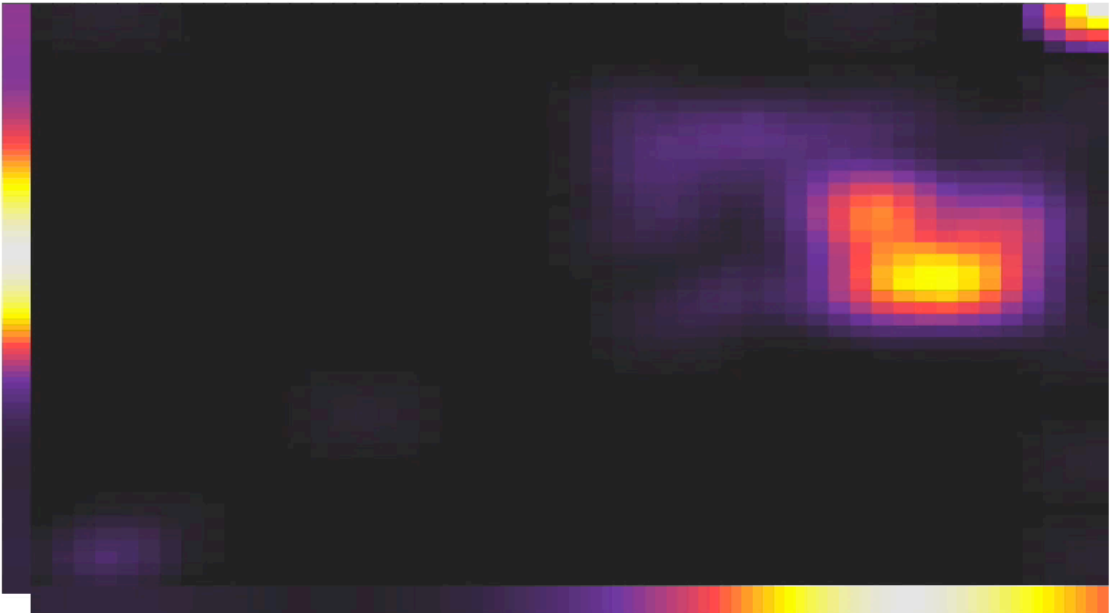
Nothing selected Use columns Custom column 202 total rows

| ID | Tool | Substrate x        | Substrate y        |
|----|------|--------------------|--------------------|
| 1  |      | 0.7781874673773234 | 0.6599116204341688 |
| 2  |      | 0.833543808403423  | 0.746030374446     |
| 3  |      | 0.6543344226852987 | 0.6882546059375454 |
| 4  |      | 0.6195678131023674 | 0.6306212655413835 |
| 5  |      | 0.6486536880495332 | 0.7644257229555012 |
| 6  |      | 0.7791129291856689 | 0.5979152983567378 |
| 7  |      | 0.7231352091463779 | 0.721192957030748  |
| 8  |      | 0.792529598930497  | 0.6681219371370225 |
| 9  |      | 0.68554642297569   | 0.7644474175098513 |

III-V Strain Compensation Calculator

x:

y:



The heatmap displays a strain distribution on a dark background. A prominent feature is a bright yellow and orange region in the upper right quadrant, indicating high strain. This region is surrounded by a purple and blue gradient, suggesting a transition to lower strain levels. The overall shape of the high-strain region is somewhat irregular, with a central peak and surrounding diffuse areas.



# IDENT: Data Exploration & Tool Execution

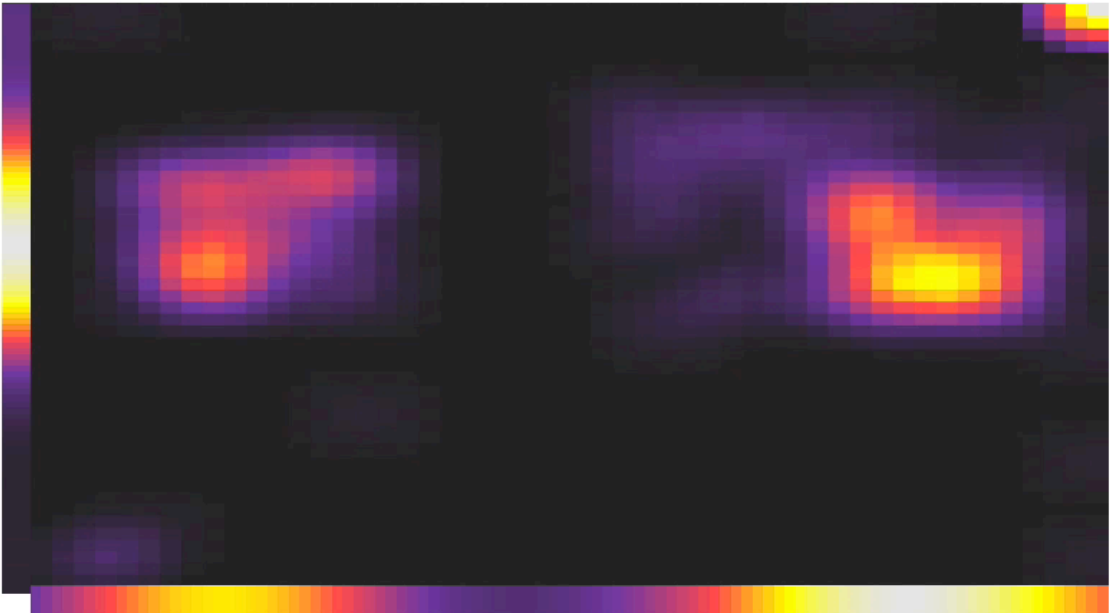
Nothing selected Use columns Custom column 302 total rows

| ID | Tool | Substrate x        | Substrate y        |
|----|------|--------------------|--------------------|
| 1  |      | 0.7781874673773234 | 0.6599116204341688 |
| 2  |      | 0.833543808403423  | 0.746030374446     |
| 3  |      | 0.6543344226852987 | 0.6882546059375454 |
| 4  |      | 0.6195678131023674 | 0.6306212655413835 |
| 5  |      | 0.6486536880495332 | 0.7644257229555012 |
| 6  |      | 0.7791129291856689 | 0.5979152983567378 |
| 7  |      | 0.7231352091463779 | 0.721192957030748  |
| 8  |      | 0.792529598930497  | 0.6681219371370225 |
| 9  |      | 0.68554642297569   | 0.7644474175098513 |

III-V Strain Compensation Calculator

x:

y:

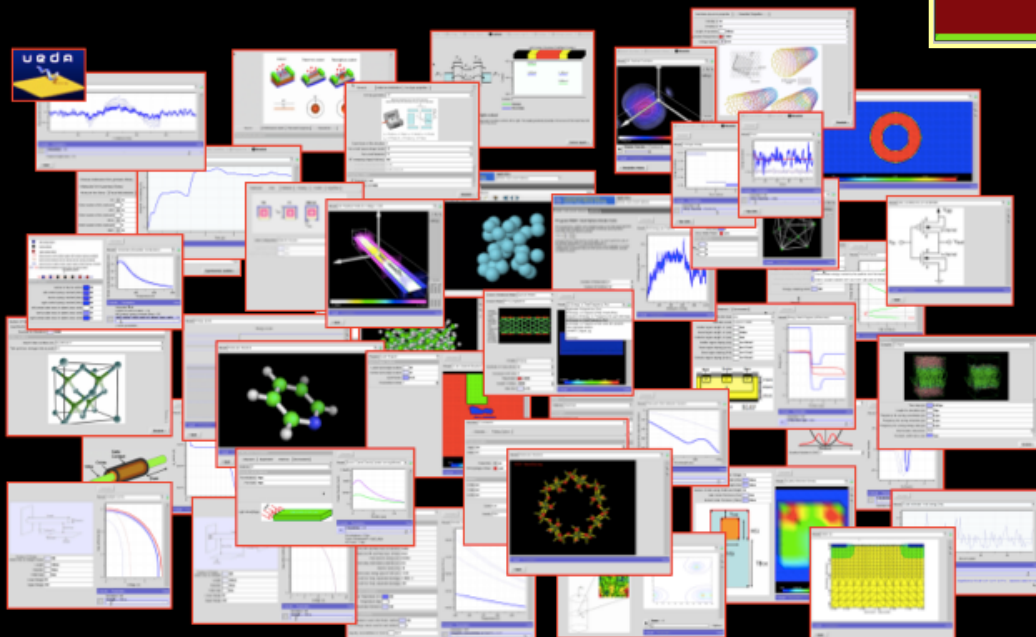


The heatmap displays a 2D distribution of strain values. The color scale ranges from dark purple (low strain) to bright yellow (high strain). Two distinct regions of high strain (yellow/orange) are visible, one on the left and one on the right, both surrounded by lower strain regions (purple/blue). The overall shape is roughly rectangular with some internal structure.

# nanoHUB

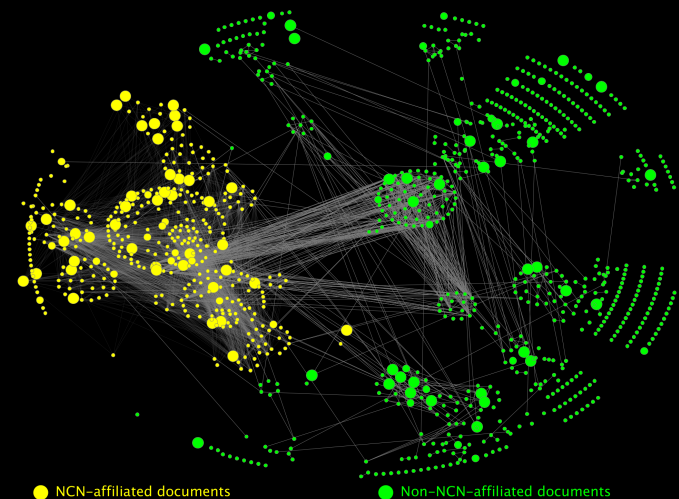
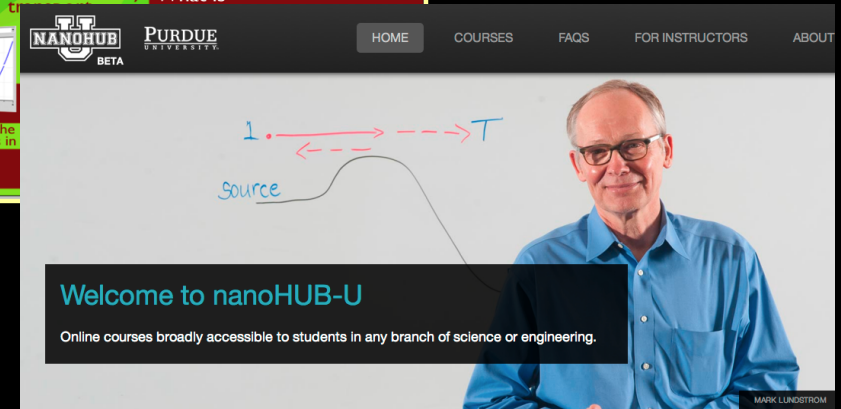
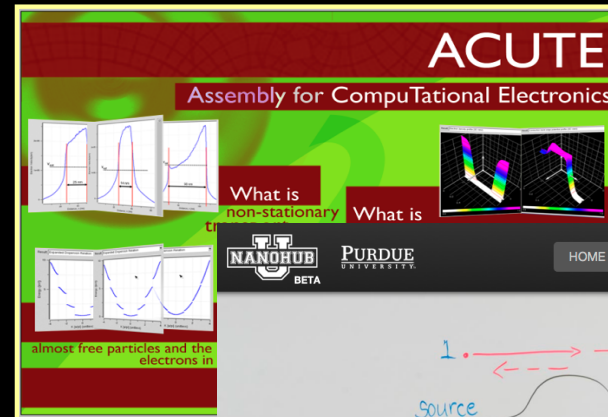
## Research in the cloud

- 400+ simulation tools
- 2,500 online seminars



## Education

- nanoHUB-U
- 500+ teaching materials



● NCN-affiliated documents

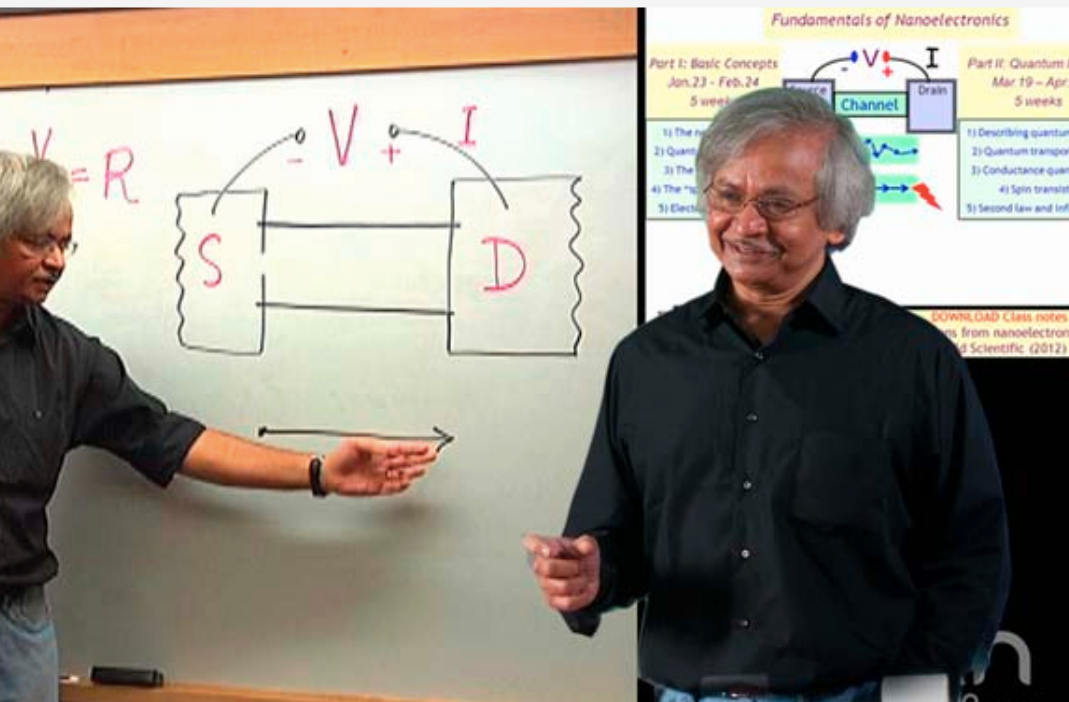
● Non-NCN-affiliated documents

\* Small dots represent papers with relatively low secondary citations, medium dots indicate papers with potential to influence h-index, large dots represent papers affecting the h-index

## Global collaboration & community

*"Truly a fabulous learning experience."*

— past nanoHUB-U student



## LATEST ONLINE COURSES

### Organic Electronic Devices (edX)

Dr. Bryan Boudouris, Assistant Professor of Chemical Engineering, Purdue University

Enroll now for the **February 12th** offering!

### Fundamentals of Nanoelectronics: Basic Concepts, 2nd Edition (edX)

Dr. Supriyo Datta, Professor of Electrical and Computer Engineering, Purdue University

Enroll now for the **March 26th** offering!

*For both these courses, the initial instructor led offering will be hosted on edX.org where you can earn a certificate. Once the initial edX offering is complete, the course be added to nanoHUB-U for self-paced studies.*

## SELF-PACED COURSES

Learn at your own pace.

## INSTRUCTOR-LED SHORT COURSES

Interact with nanoHUB-U profs and earn a certificate of completion

Coming Soon:

[Organic Electronic Devices \(edX\)](#)

[Fundamentals of Nanoelectronics: Basic Concepts, 2nd Edition \(edX\)](#)

## Q & A Forums

Faculty-curated Q & A pages for specific topics.

Visit a particular forum to get answers or to submit a question.

### Transport Fundamentals - Bottom-Up Approach

### Transport Fundamentals - Ballistic Conductance and Conductivity

### Transport Fundamentals - NEGF

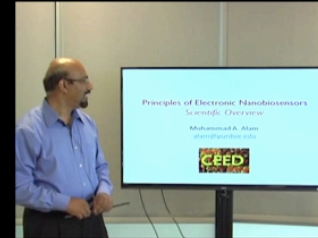


# nanoHUB-U courses related to materials

- A forum for evolving, original viewpoints that should become mainstream
- Focus on seniors, beginning grad students, working engineers
- Designed to “transcend disciplines” and be broadly accessible (no long list of prerequisites)
- Short but not too short (5 weeks) and not superficial
  - 5 20-minute lectures per week

# nanoHUB-U / edX in numbers

- Full courses: 15
- Short courses: 2
- Total enrollment: 12,634
  - ~10% from Industry
  - 180 companies represented
  - 80+ countries



## Principles of Electronic Nanobiosensors Scientific Overview

Muhammad A. Alam  
[alam@purdue.edu](mailto:alam@purdue.edu)



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### Fundamentals of Nanoelectronics, Part B: Quantum Transport

Explore quantum transport in nanoscale devices and spintronics in this introductory nanotechnology course.

Join Now  
Started on October 8, 2015

**Enroll Now**

I would like to receive email from Purdue University and learn about its other programs.

"This MOOC is one of the best. Exceptional in all regards." – Student from Part A

**PURDUE UNIVERSITY**

**About this course** 0 Reviews 0/5 ★★★★★

Nanoelectronic devices are an integral part of our life, including the billion-plus transistors in every smartphone, each of which has an active region that is only a few hundred atoms in length.

This nanotechnology course explains the fundamentals of nanoelectronics and mesoscopic physics.

[See more](#)

**What you'll learn**

- Introduction to the Tight-binding Method

Length: 8 weeks  
Effort: 5 - 6 hours/week  
Price: FREE  
Add a Verified Certificate for \$50  
Institution: PurdueX  
Subject: Electronics  
Level: Intermediate

- Full courses: 7
- Total registrations 51,160
- 27% high school education
- 38% college degree
- 32% advanced degree
- 40% from Industry

# Workshop: UQ for materials modeling

## IMA Hot Topics Workshop Uncertainty Quantification in Materials Modeling

July 28-31, 2015

Please note, this workshop will take place at Purdue University in West Lafayette, Indiana.



Program Application closed // Abstracts and Talk Materials // Poster //

### Organizers

|                     |  |
|---------------------|--|
| Mark Benedict       | US Air Force Research Laboratory               |
| Andrea Browning     | The Boeing Company                             |
| Stephen Christensen | The Boeing Company                             |
| Andrew Dienstfrey   | National Institute of Standards and Technology |
| Paul Patrone        | University of Minnesota, Twin Cities           |
| Frederick Phelan    | National Institute of Standards and Technology |
| Alejandro Strachan  | Purdue University                              |

- Six half-day hands-on workshop session
  - All simulations using nanoHUB
- Half-day cutting-edge research talks

POWERED BY nanoHUB.org

Alejandro Strachan strachan@purdue.edu

### Introduction to Uncertainty Quantification

Course overview Offering: 2015 Summer School Section: Default

Manage the content of the outline here. Build outline

- Unit 1: (Strachan) Uncertainty Quantification Across Scales and Physics: Towards Predictive Materials
  - Lectures
    - L1.1: Introduction to UQ in Materials and Model Calibration
    - L1.2: Uncertainty Propagation in Multiscale, Multiphysics Simulations
    - L1.3: nanoHUB Workspace, Uncertainty Propagation with PUQ, and Functional Uncertainty Quantification



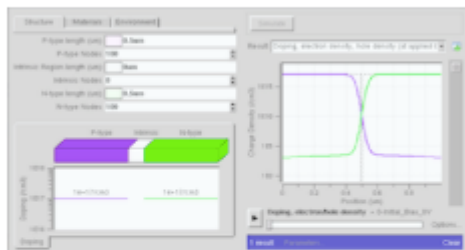
- 25% of participants from Industry: Boeing, Dow Chemical, Intel, Schrodinger, Inc., Corning Inc., Solvay Cytec

Innovate, educate, engage



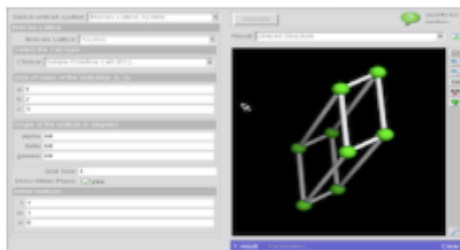
# Simulation-enhanced learning

## Most Popular Simulation Tools for Education



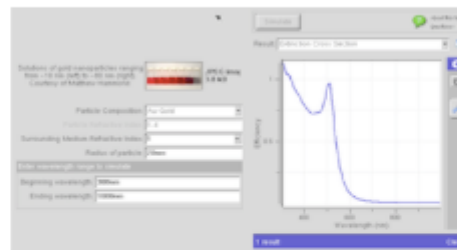
PN Junction Lab

- [Launch Tool.](#)



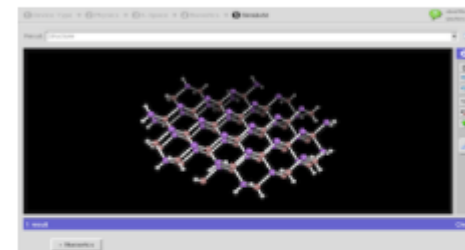
Crystal Viewer Tool

- [Launch Tool.](#)



Nanosphere Optics Lab

- [Launch Tool.](#)



Band Structure Lab

- [Launch Tool.](#)

[see more](#)

## NCN Supported Learning Packages



nanoHUB-U



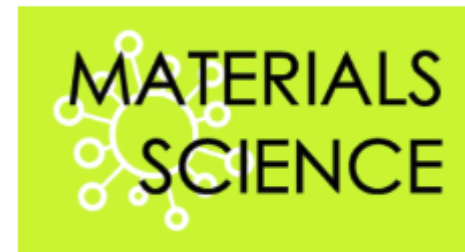
General Chemistry Simulations

- [Collection materials and overview.](#)  
- [Simulation Page.](#)



Semiconductor Simulations

- [Collection materials and overview.](#)  
- [Simulation Page.](#)



Materials Science Simulations

- [Collection materials and overview.](#)



# Learning about materials using simulations

<https://nanohub.org/topics/LearningModulePlasticityMD>

nanoHUB.org - Wiki: Learning Module: Atomic Picture of Plastic Deformation in Metals

1050 New Messages

Search

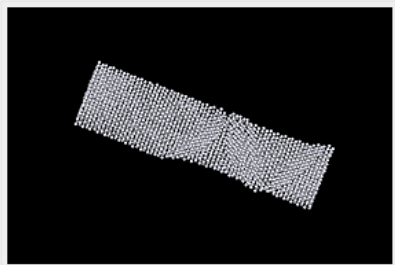
Home Resources Members Explore nanoHUB-U Partners About Support

Home > Topics > Learning Module: Atomic Picture of Plastic Deformation in Metals

## Learning Module: Atomic Picture of Plastic Deformation in Metals

by Joseph M. Cychosz, Alejandro Strachan

Article Edit Comments History



The main goal of this learning module is to introduce you to plastic deformation in crystalline metals and help them develop a more intuitive understanding of it. The image on the right shows plastic deformation of a metallic nanowire.

The module consists of:

- Two introductory lectures (50 minutes each) available online as audiovisual presentations
  - [Overview Lecture](#)
  - [Prelab Lecture](#)

nanoHUB.org - Resources: Tools: nano-Materials Simulation Toolkit: Session: 403718 "nano-Materials Simulation Toolkit"

https://nanohub.org/tools/matsimtk/session/403718

Result: Structure at 2.0ps

1 result Parameters Clear

< Input

# Assessing students learning



Advances in Engineering Education



WINTER 2013

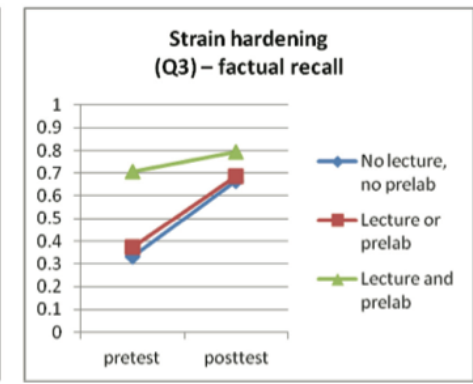
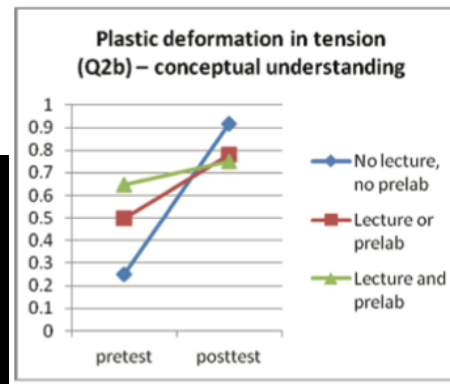
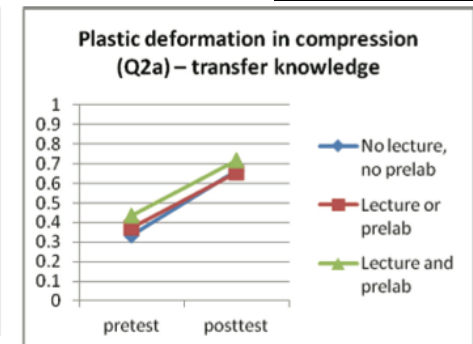
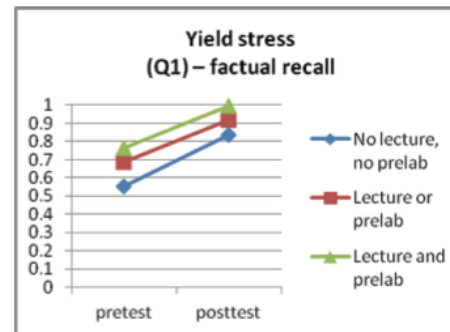
## Lectures and Simulation Laboratories to Improve Learners' Conceptual Understanding

SEAN P. BROPHY  
Engineering Education

ALEJANDRA J. MAGANA  
Computer and Information Technology

AND

ALEJANDRO STRACHAN  
Materials Engineering  
Purdue University  
West Lafayette, IN

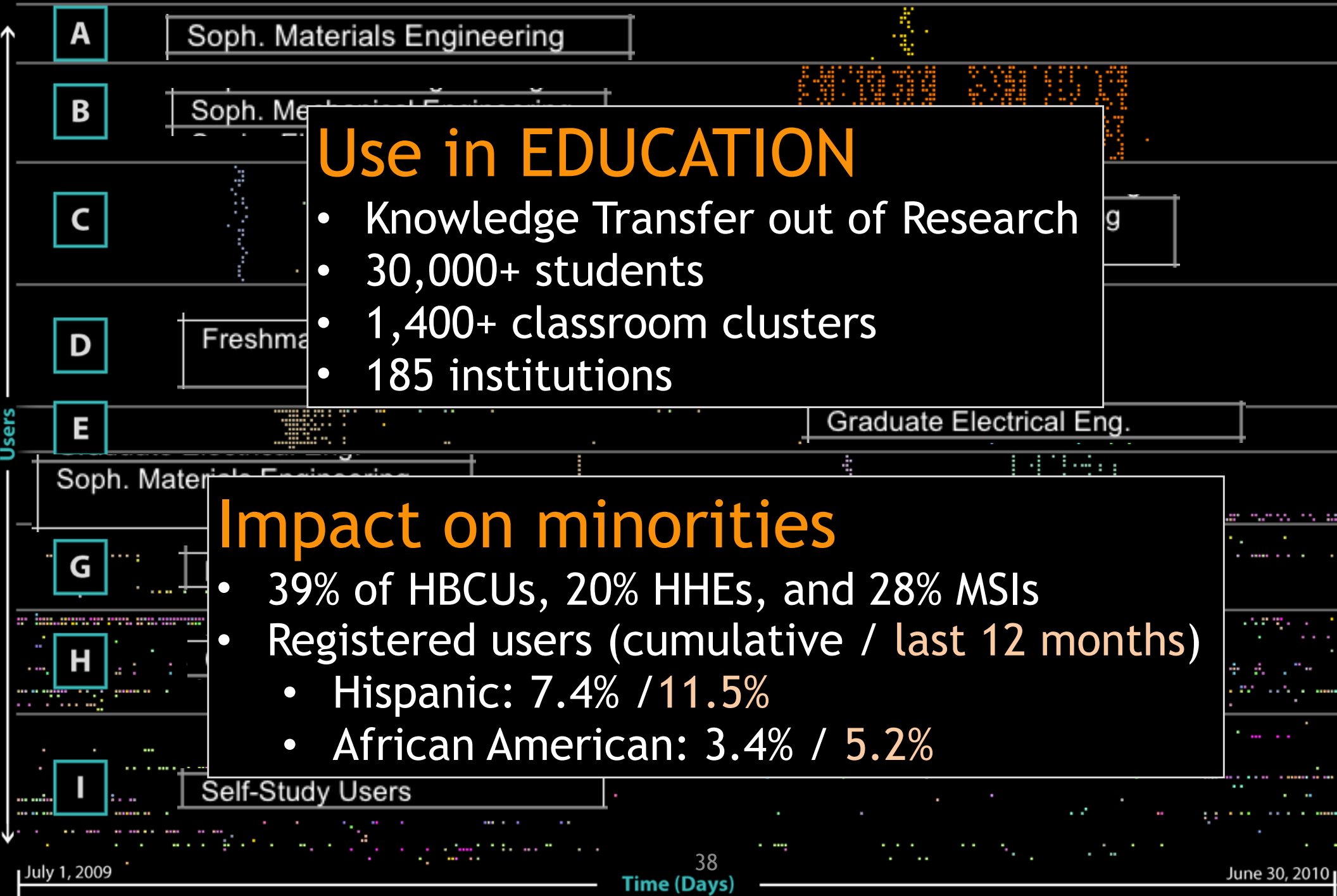


# nanoHub User Behavior

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# nanoHUB usage statistics





# Empowering communities

Industry

Researchers

Instructors

Students

1.4 M visitors 12,000+ simulation users per year



# Join the materials group!

[nanohub.org/groups/materials](https://nanohub.org/groups/materials)

**Materials Science** ▶ Overview

Welcome to the Materials Science group! If you are a student or practicing engineer or scientist who wants to learn more about materials science or an instructor looking for materials to use in a course, you can find resources here that include complete courses and seminars on specialized topics as well as simulation tools and learning activities that use simulations.

### Materials Courses

- nanoHUB-U
- Undergraduate
- Graduate

### Simulation-Powered Learning Activities

- [Mechanical properties](#)
- [Electronic structure and properties](#)
- [Transport, Thermodynamics and Phase Transitions](#)
- [More coming soon](#)

### Materials Simulation Tools

- [Ab Initio and Electronic Structure](#)
- [Molecular Dynamics](#)
- [Mesoscale Simulations](#)
- [Macroscopic Simulations](#)
- [Uncertainty Quantification](#)

**Phase Diagrams and Material Potential**

**Nanoscale tensile tests: MD results**

