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

Ale Strachan, Purdue University
Deputy Director, nanoHUB
strachan@purdue.edu

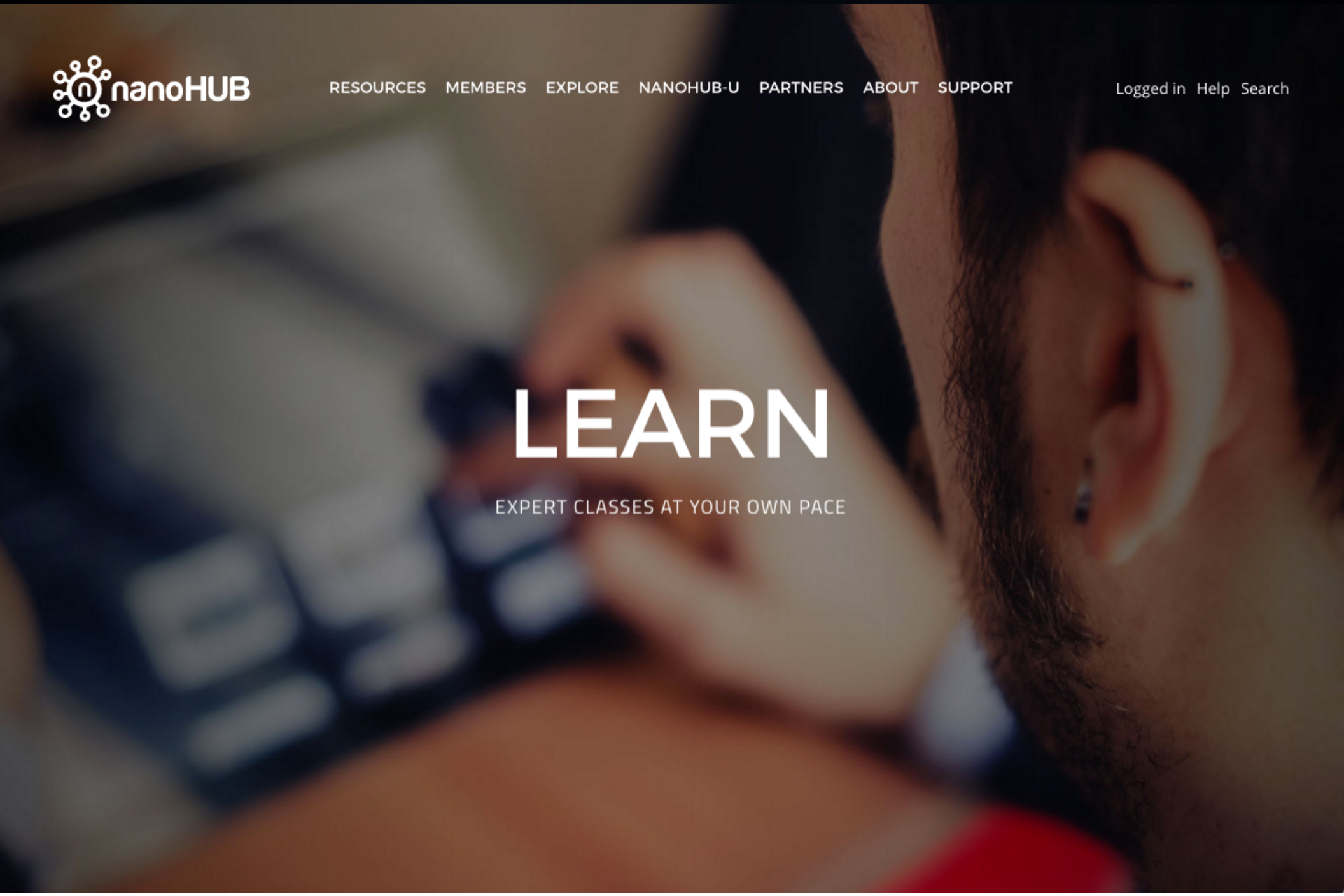
Summit on Data and Data Analytics, Evanston IL

PURDUE UNIVERSITY

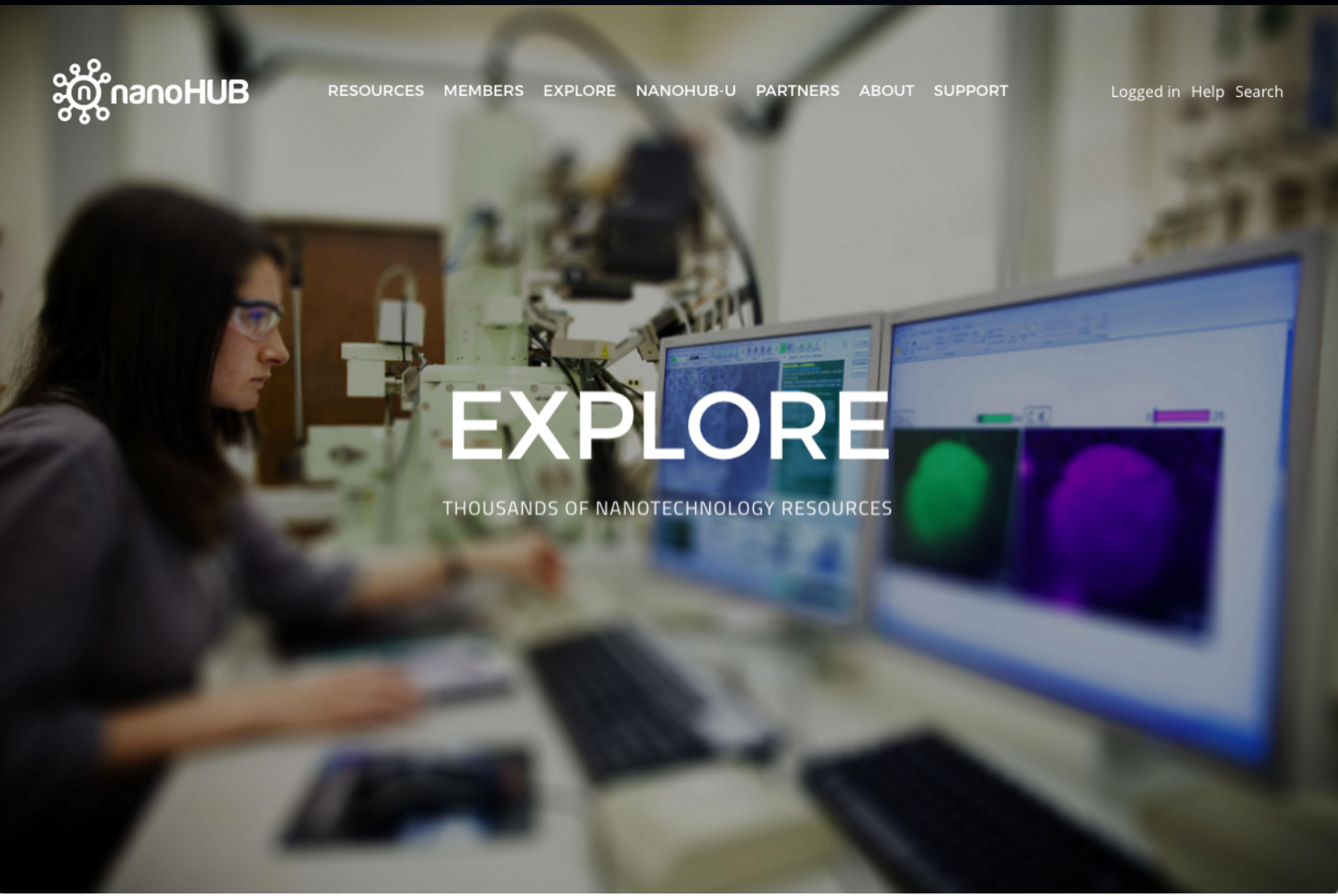
nanoHUB


nanoHUB
RESOURCES MEMBERS EXPLORE NANOHUB-U PARTNERS ABOUT SUPPORT
Logged in Help Search
NANO is HUGE
LARGEST NANOTECHNOLOGY ONLINE RESOURCE
400
simulation tools
1.4M
visitors
4500
resources
NSF
National Science Foundation
WHERE DISCOVERIES BEGIN

much more than a web site



much more than a web site



much more than a web site

nanoHUB

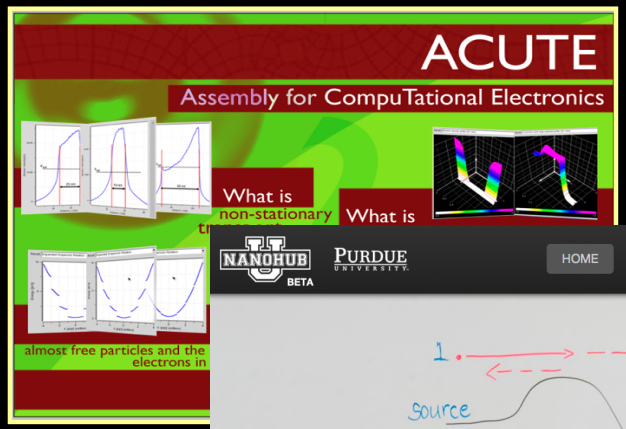
Making simulations & data universally accessible and useful

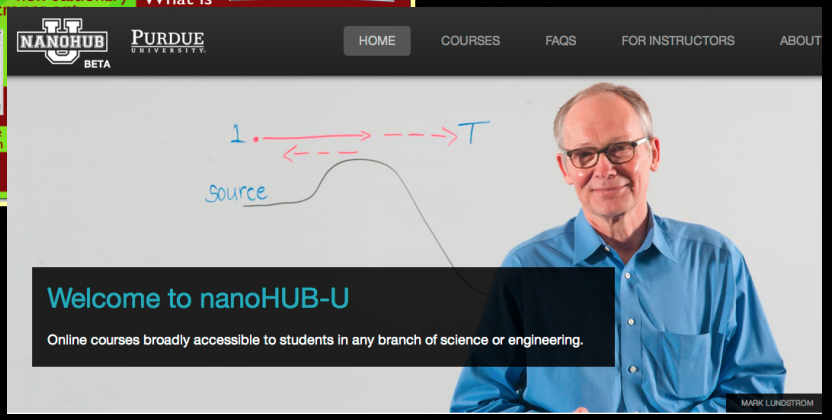
Research in the cloud

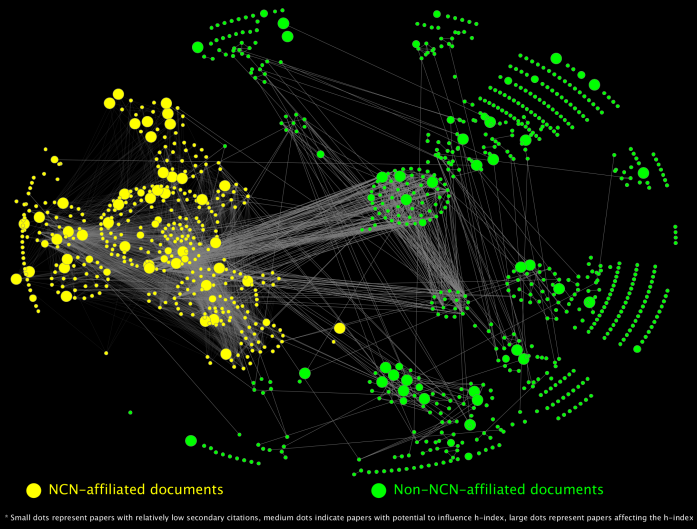
- 400+ simulation tools
- 2,500 online seminars

Education

- nanoHUB-U
- 500+ teaching materials







National Science Foundation
WHERE DISCOVERIES BEGIN

Global collaboration & community

nanoHUB



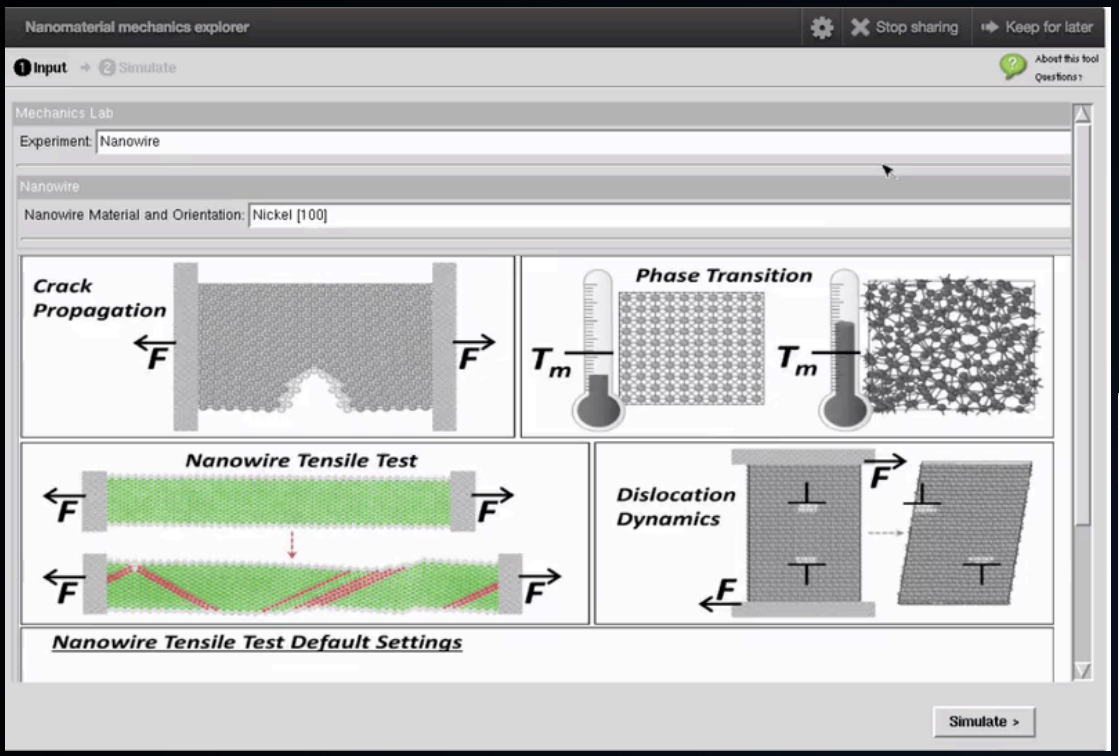

- Community driven

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



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

Innovate, educate, engage

Impact on research

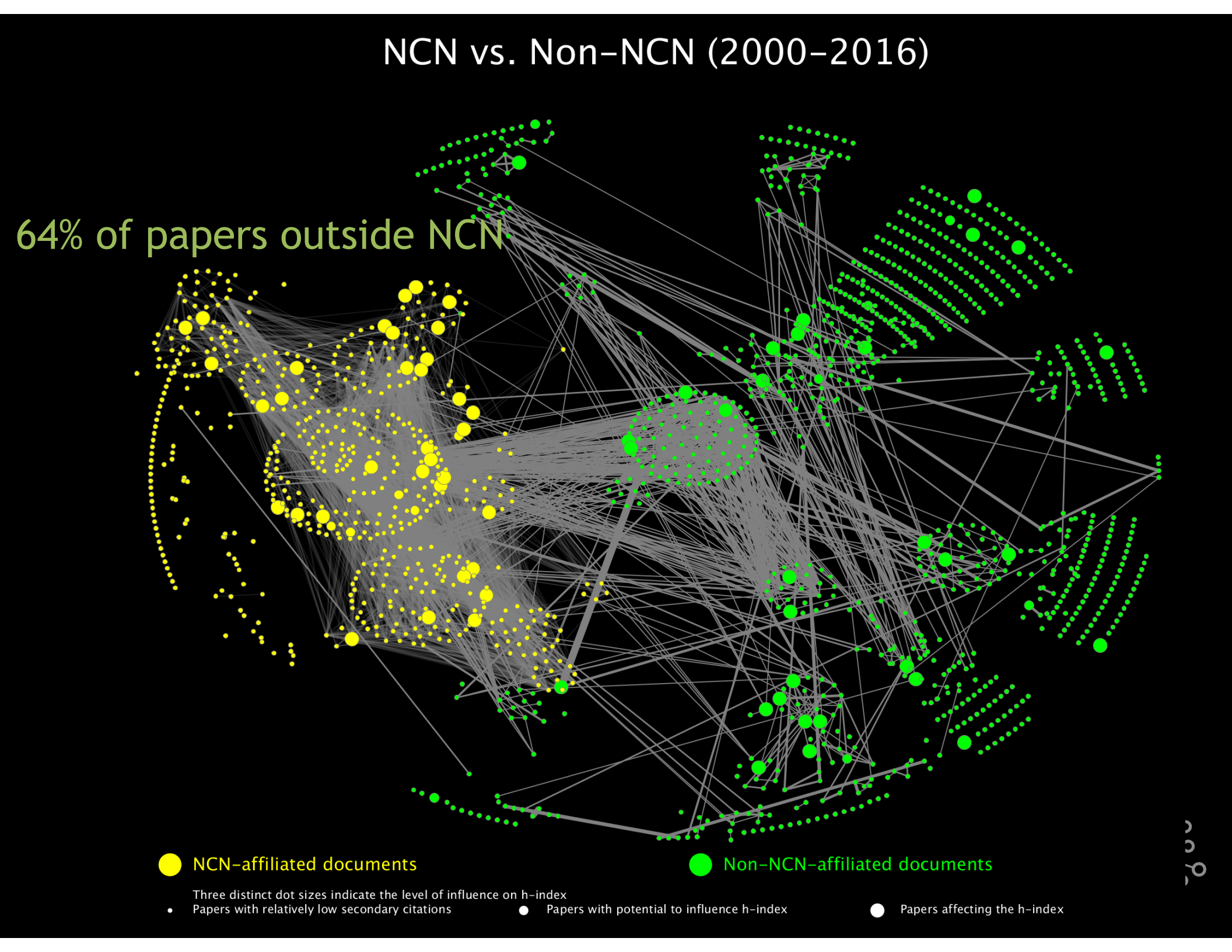
nanoHUB Citation Network (2000–2016)

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)



nanoHUB is a publisher

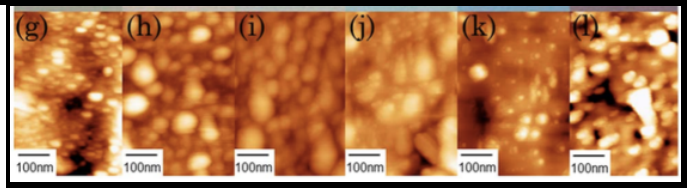
OPTICS LETTERS / Vol. 36, No. 8 / April 15, 2011

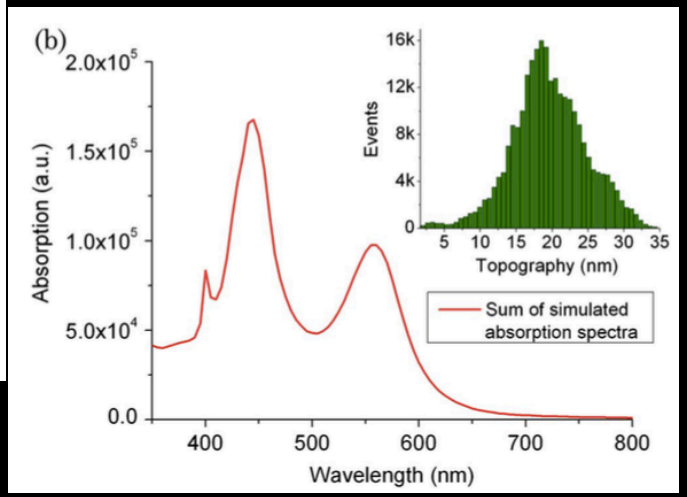
Engineering the plasmon resonance of large area bimetallic nanoparticle films by laser nanostructuring for chemical sensors

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

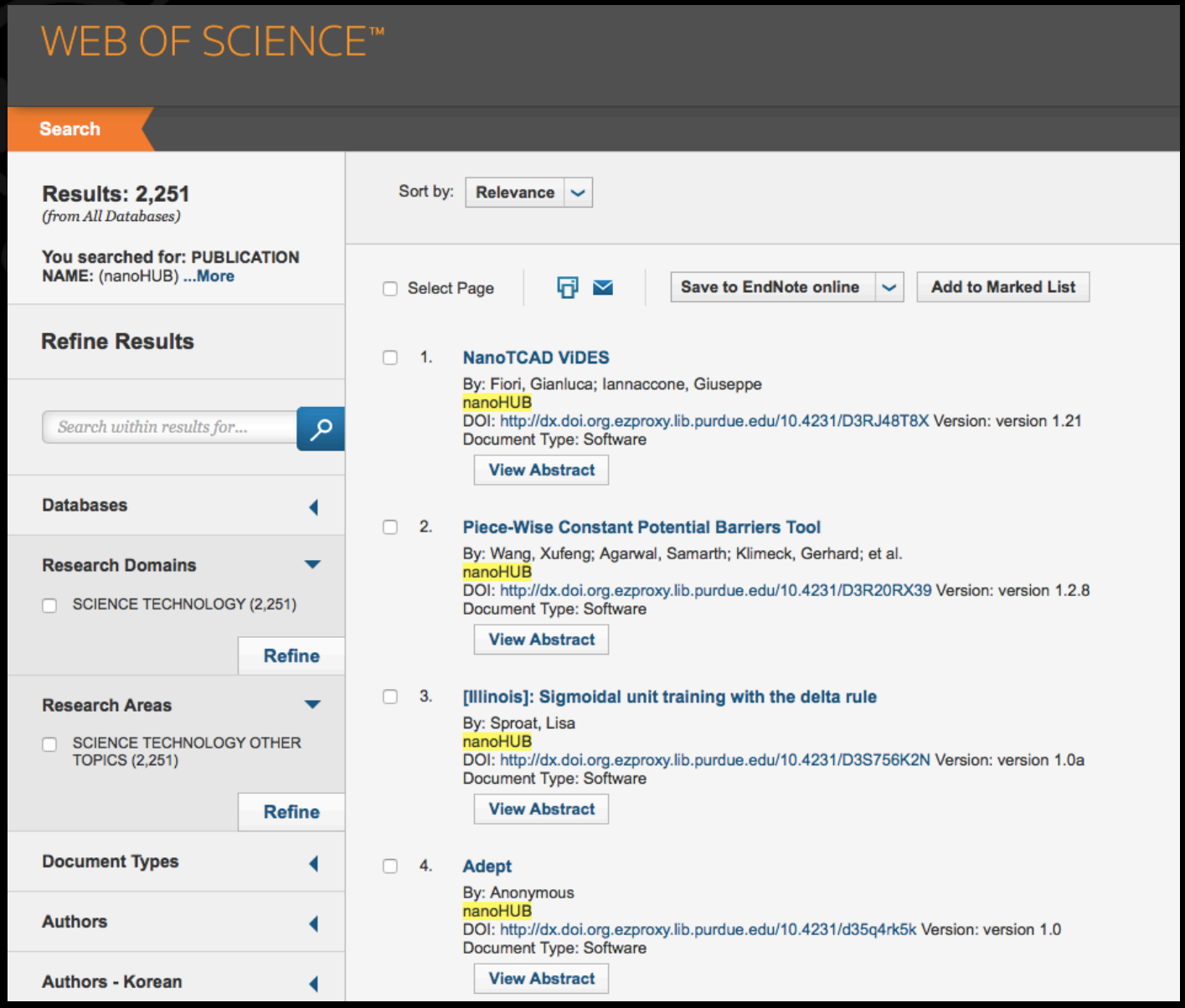
Pennsylvania State University

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

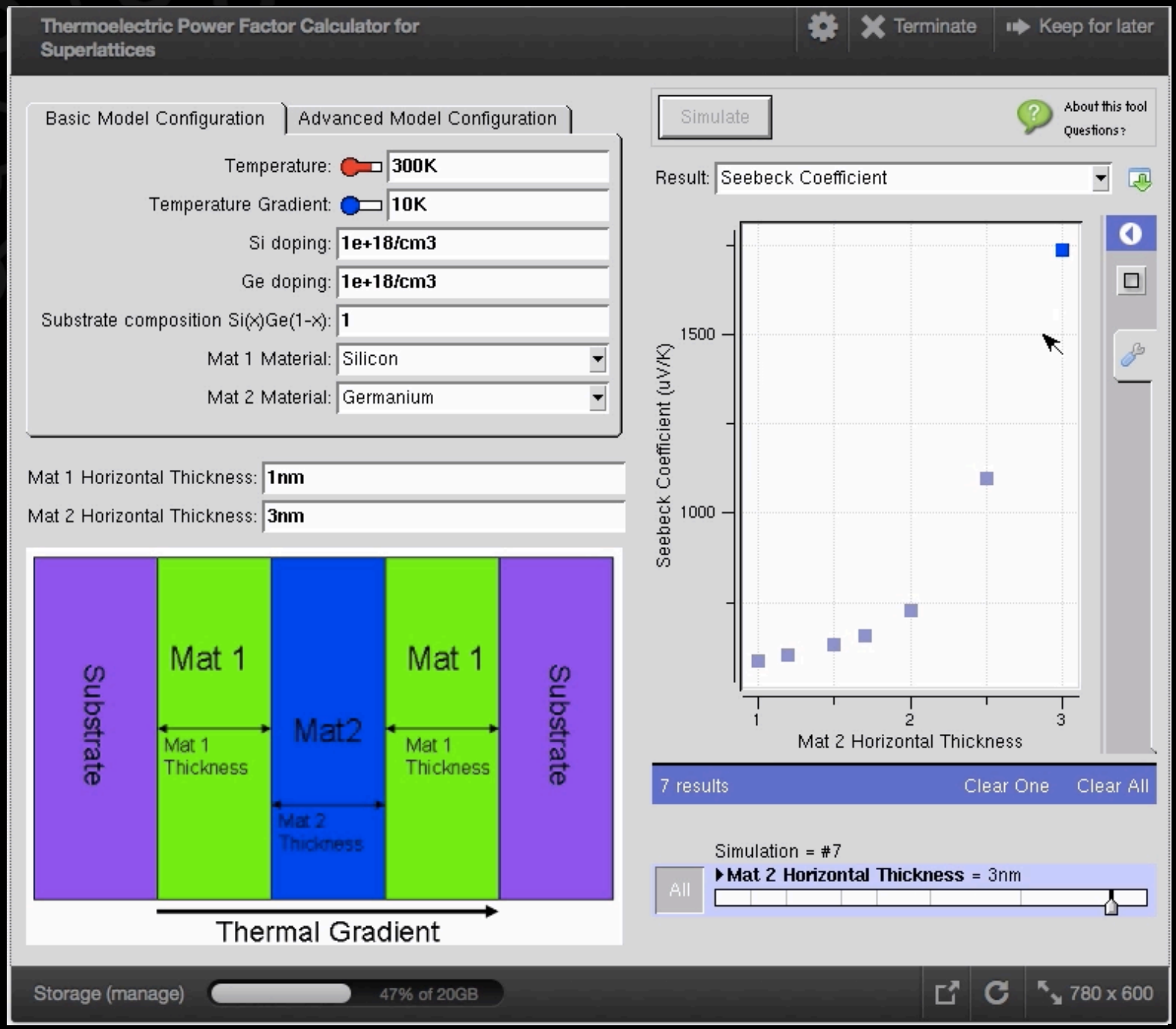
Sponsored by Penn State Center for Nanoscale Science (MRSEC)

Version	Released	DOI Handle
1.03UQ	03 May 2016	doi:10.4231/D3TH8BP1C
1.03	04 Aug 2014	doi:10.4231/D37W6765J
1.02	19 Oct 2012	doi:10.4231/D3DB7VP65
1.01	29 Apr 2010	doi:10.4231/D3PV6B66Z
1.0	29 Jan 2010	doi:10.4231/D3VX0631H

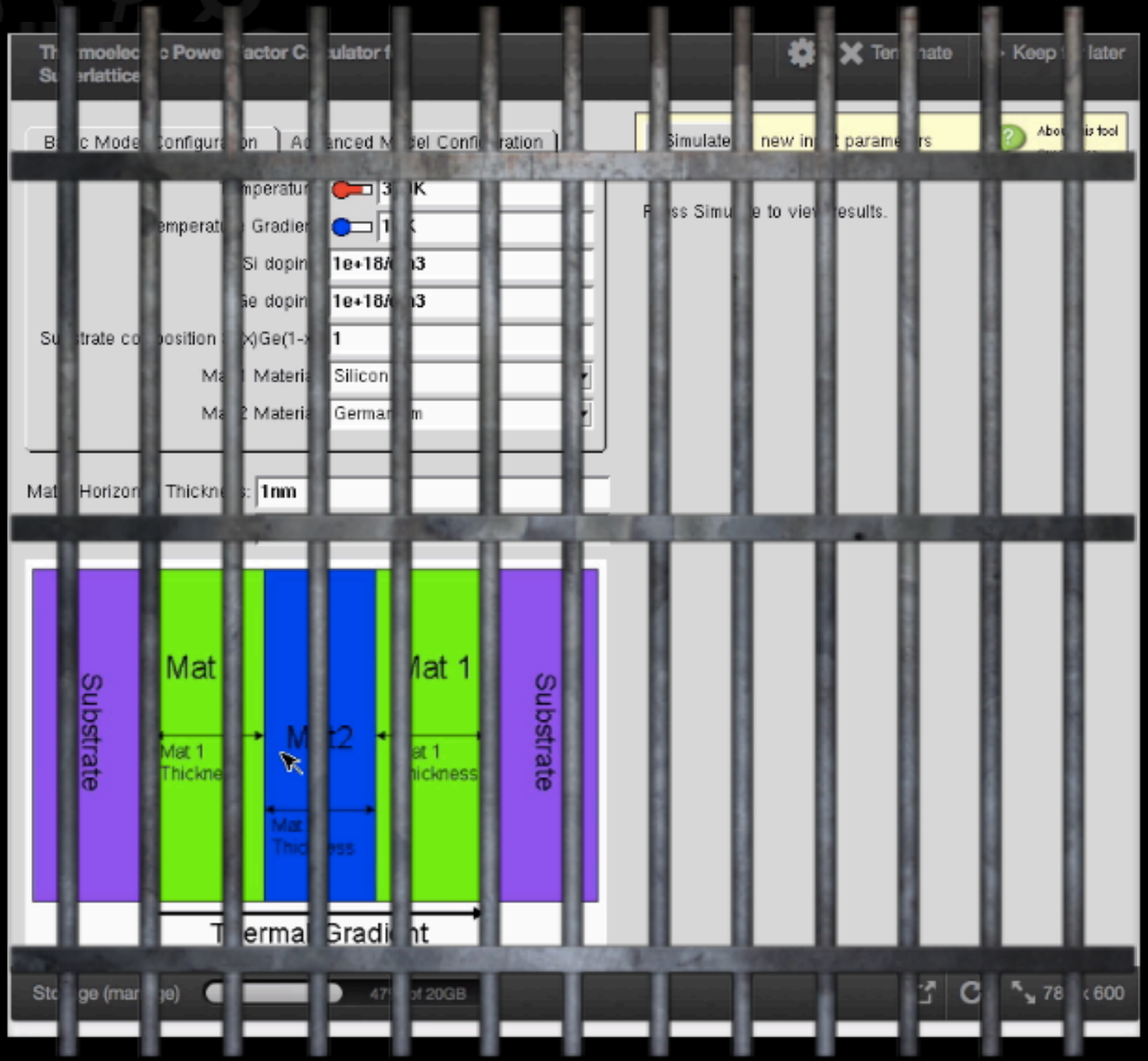
nanoHUB tools indexed by Web of Science



Re-thinking simulations



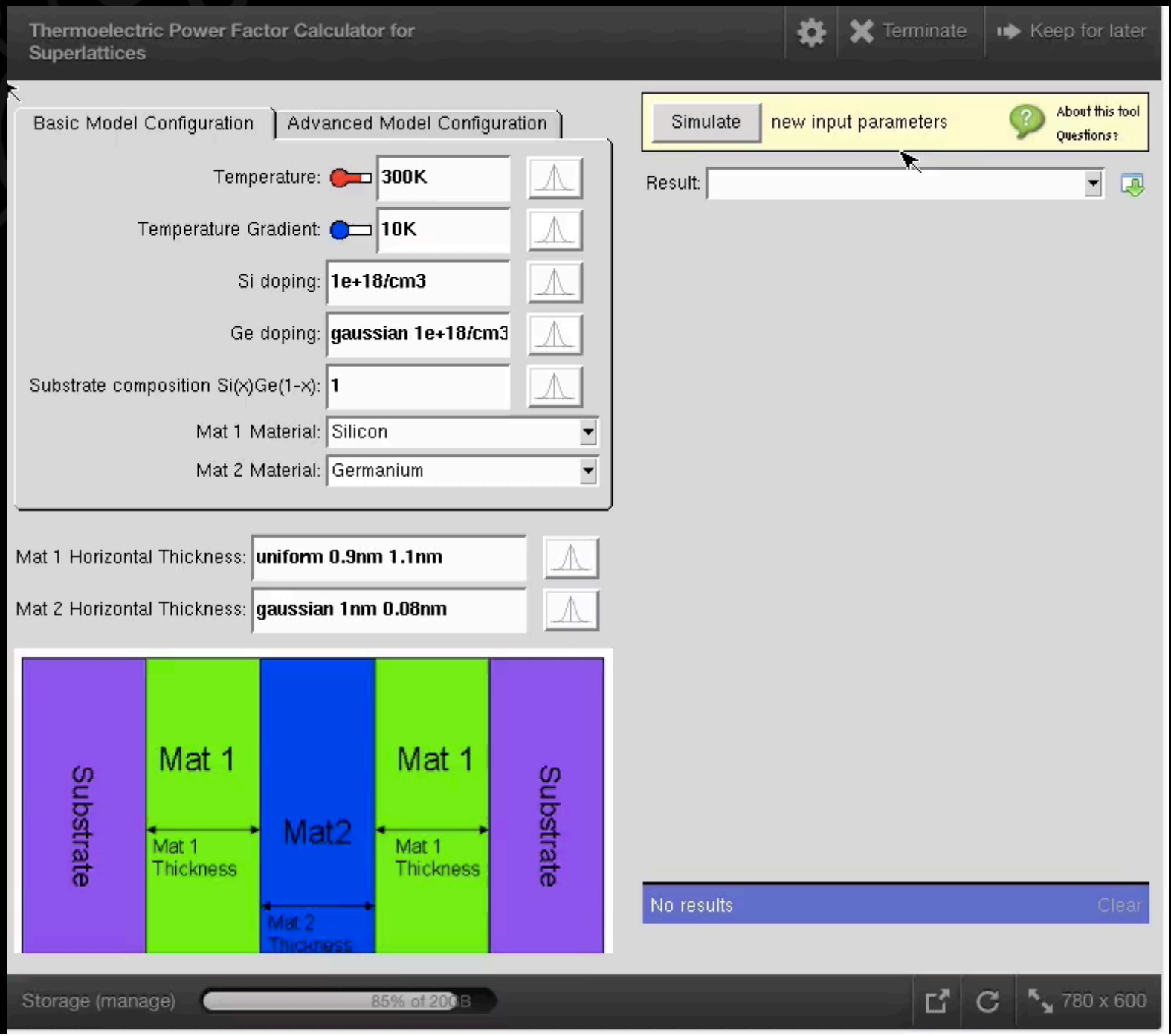
Simulation tools are limited by infrastructure



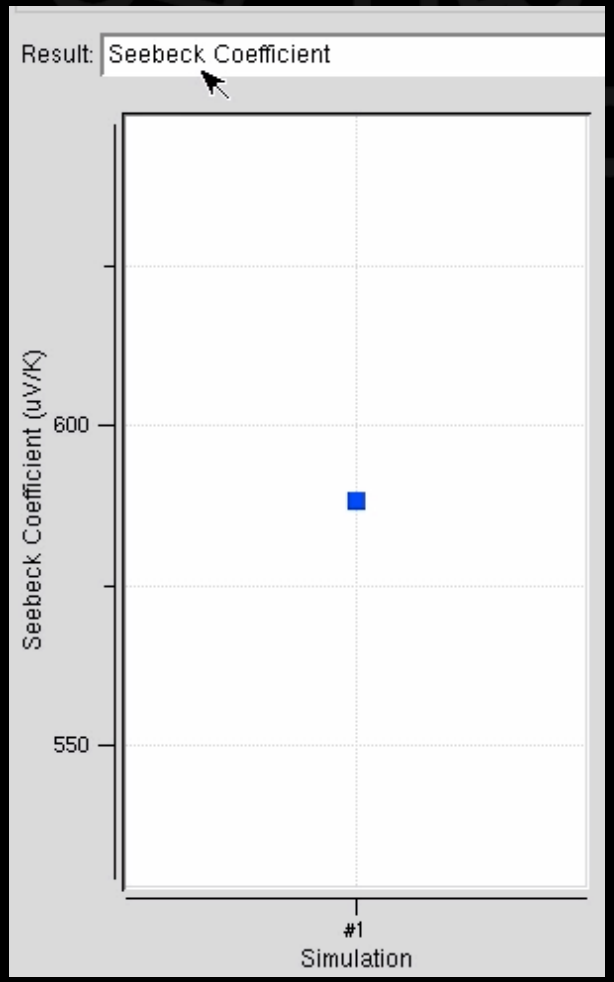
Simulation tools are limited by infrastructure

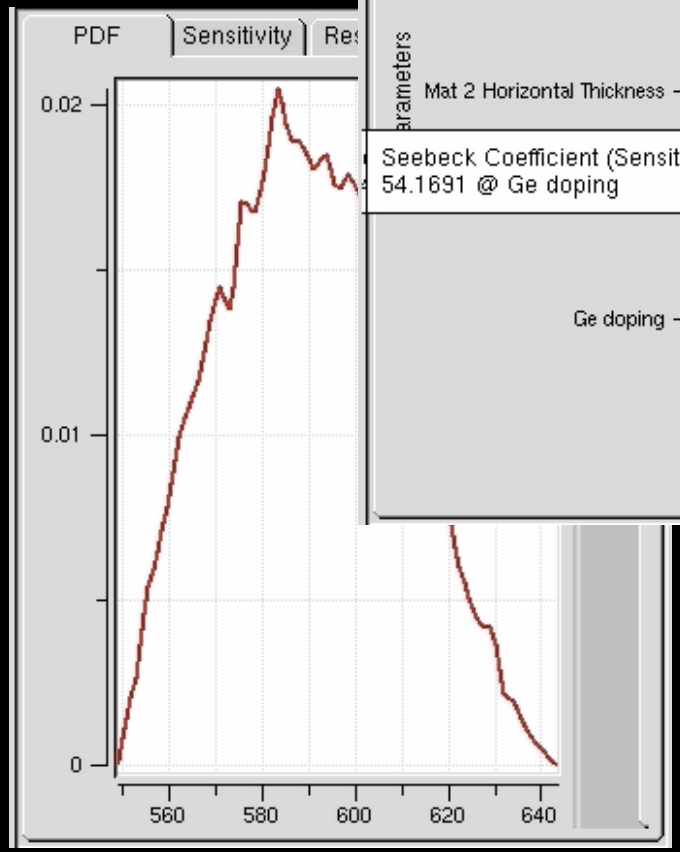
- Automatic uncertainty quantification in ALL nanoHUB tools
- New ways of executing tools - connecting tools with data exploration
- Connecting nanoHUB to other cyber-resources

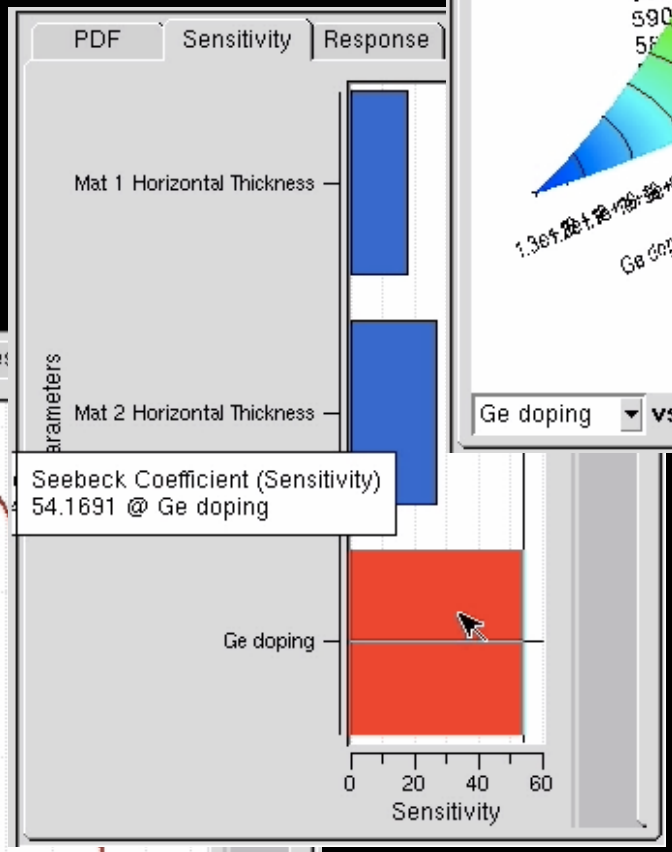
Your tool … more powerful in nanoHUB

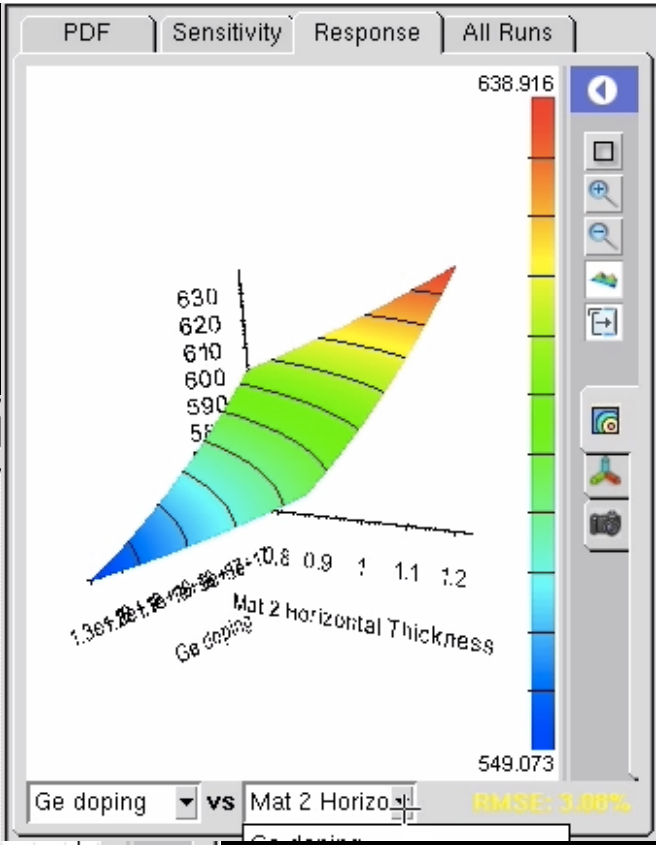


Automatic UQ in nanoHUB

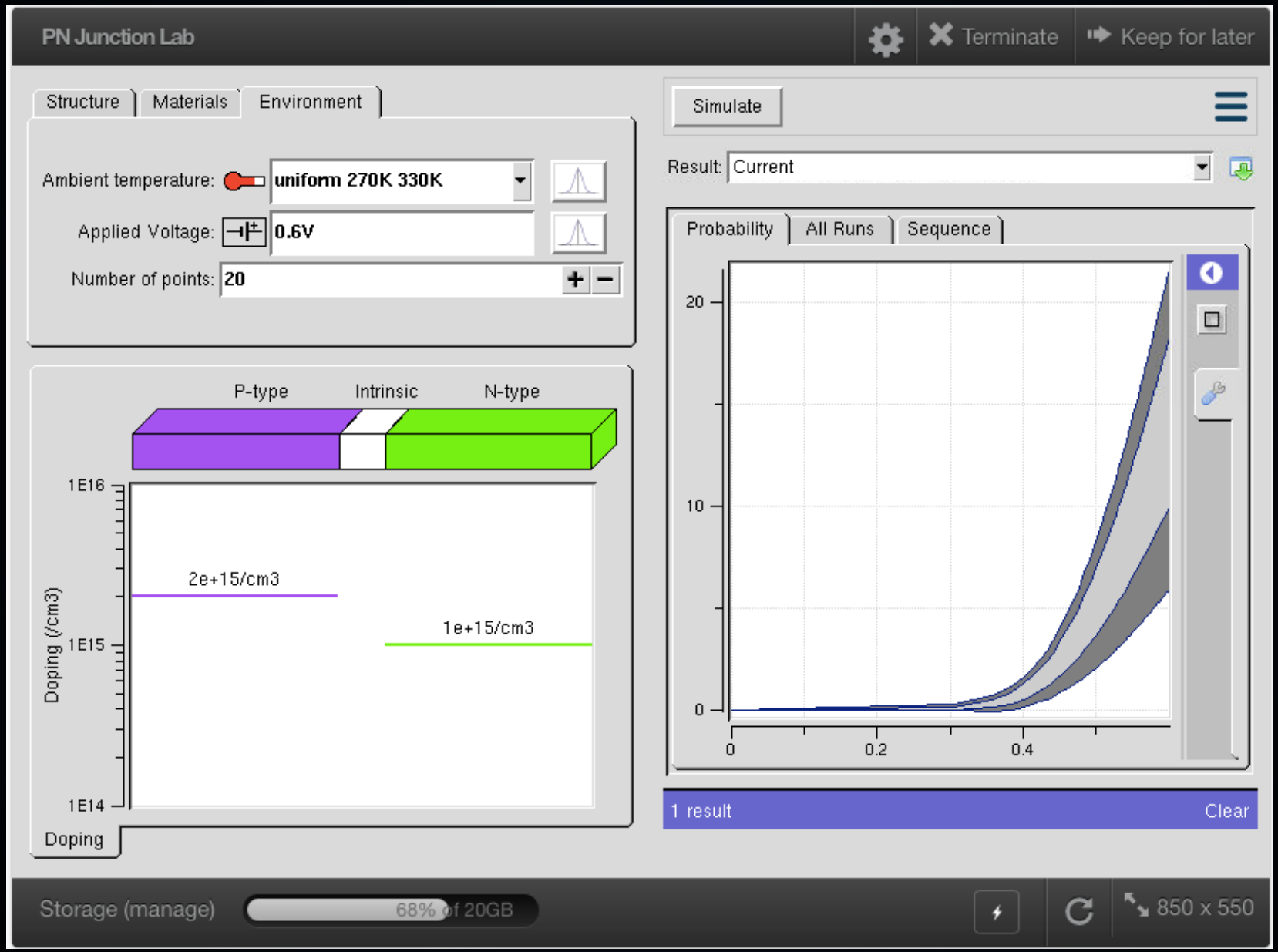






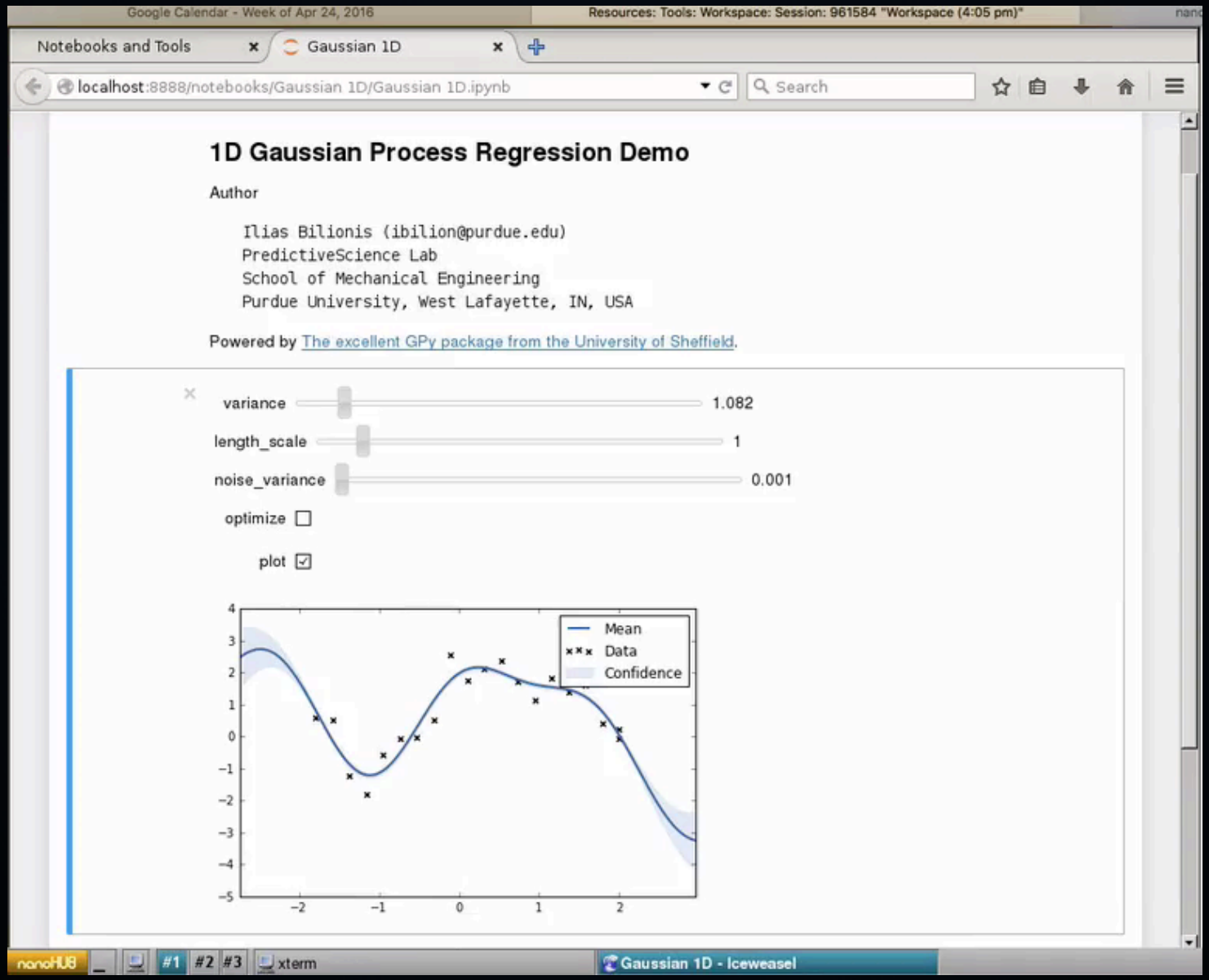


Rigorous error bars in 1D curves



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.

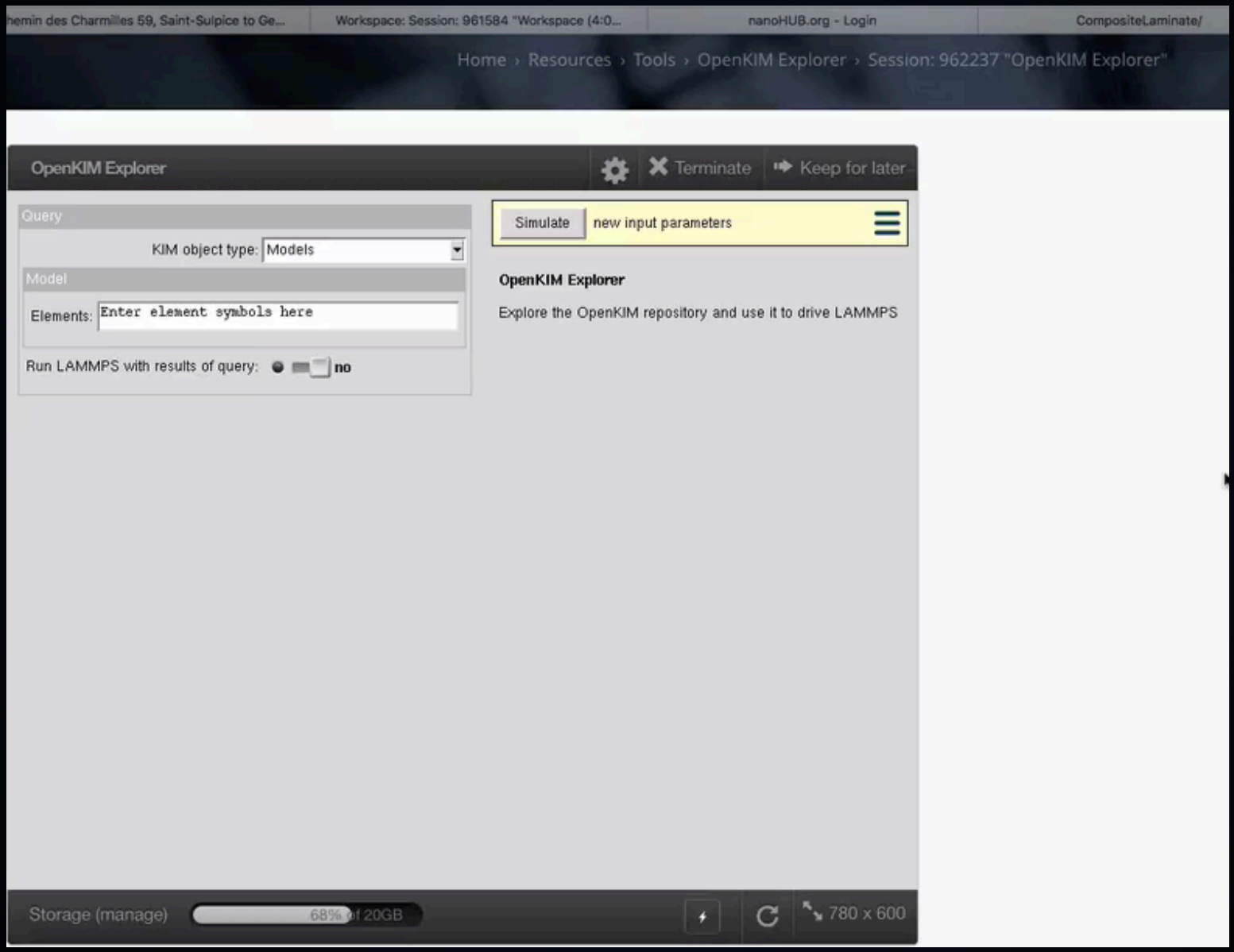
KIM Models (interatomic potentials and force fields) are software packages for describing atomic interactions that can be used with a variety of simulation codes, including LAMMPS, DL_POLY, IMD, ASE and GULP, that are compatible with the KIM API standard.

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

0 Models — 28 Models

nanoHUB

nanoHUB tool connecting to KIM

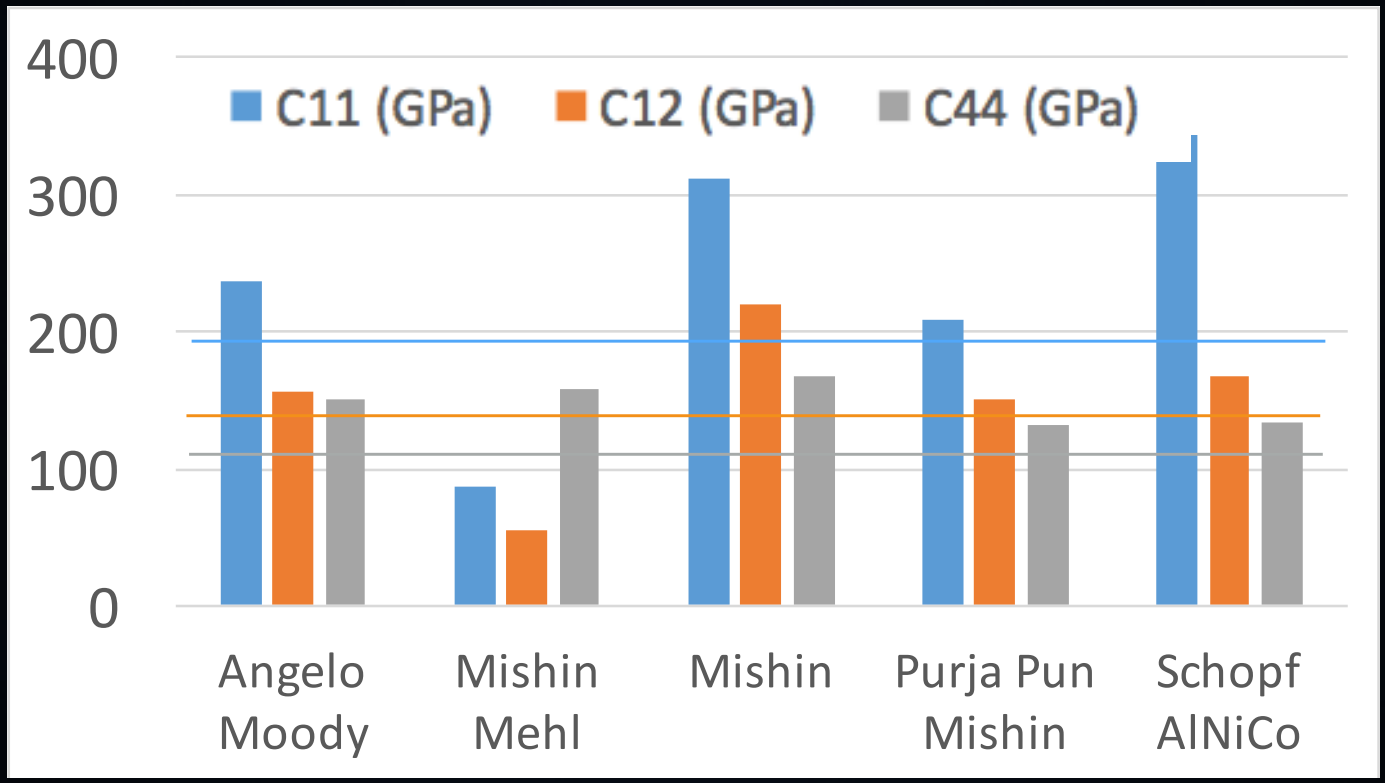


nanoHUB

openkim.org

KIM

Make a decision about your research

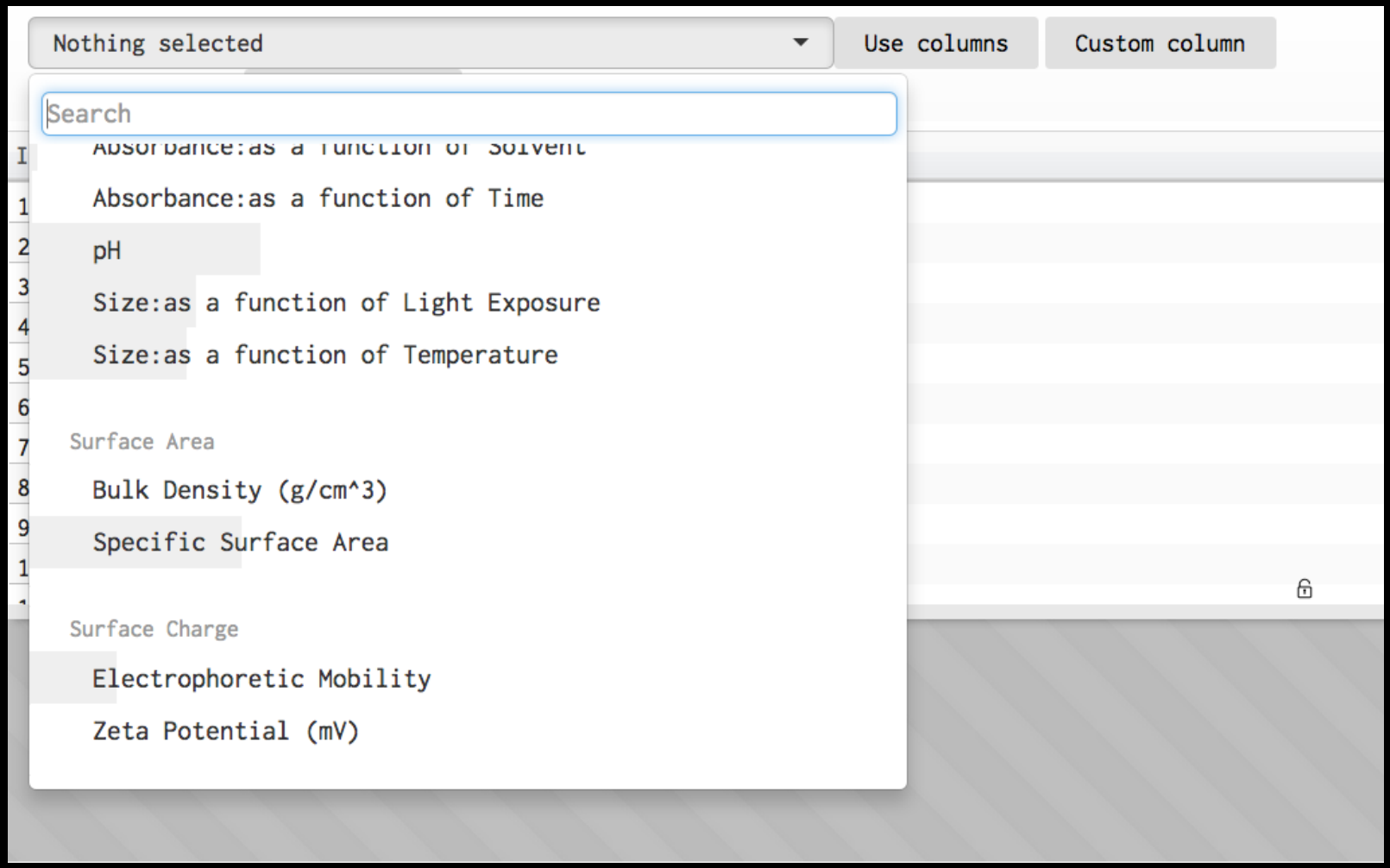


IDENT: sparse data exploration tool

& Navigation Tool

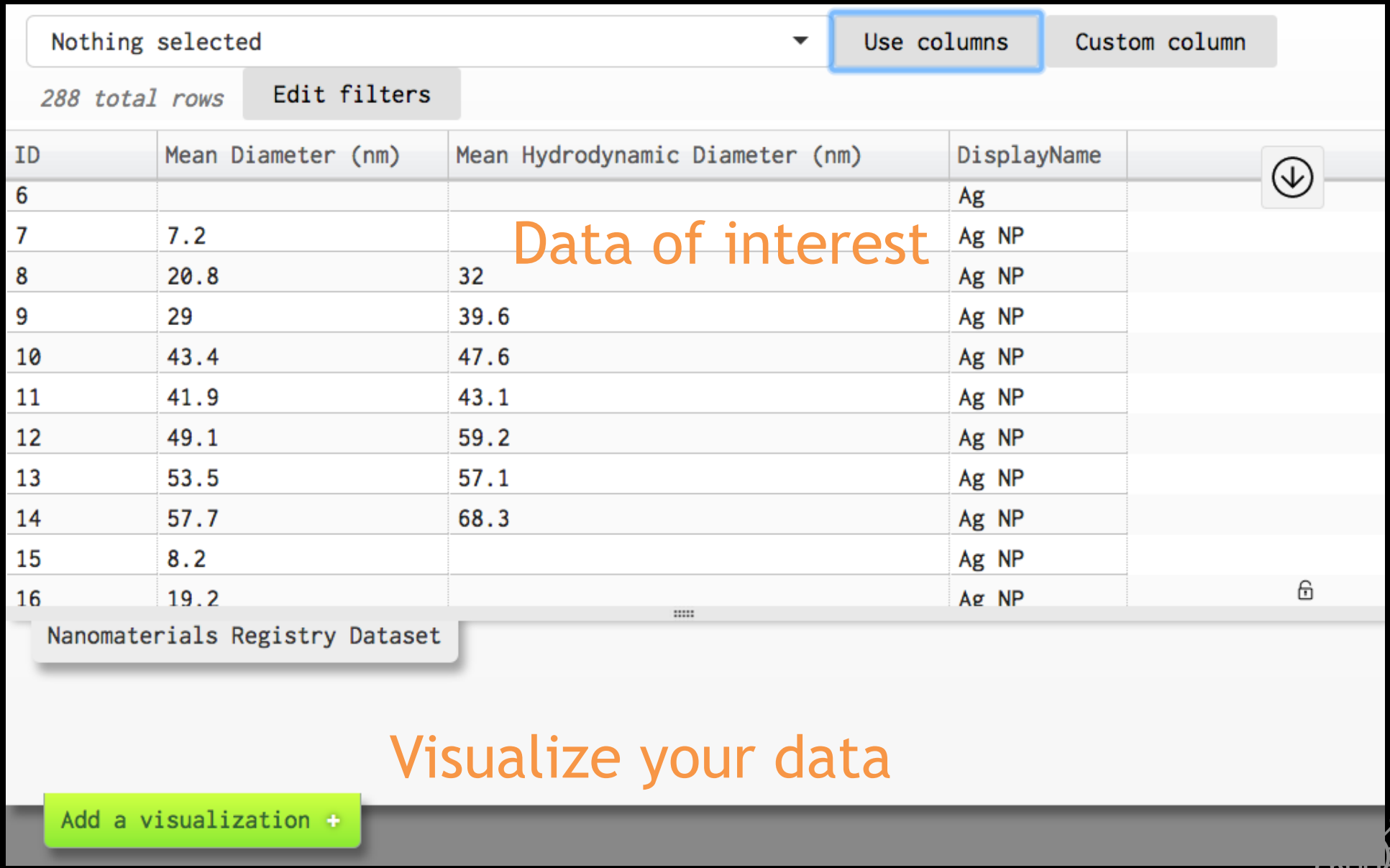
Interactive Data Exploration

for Nano Technology

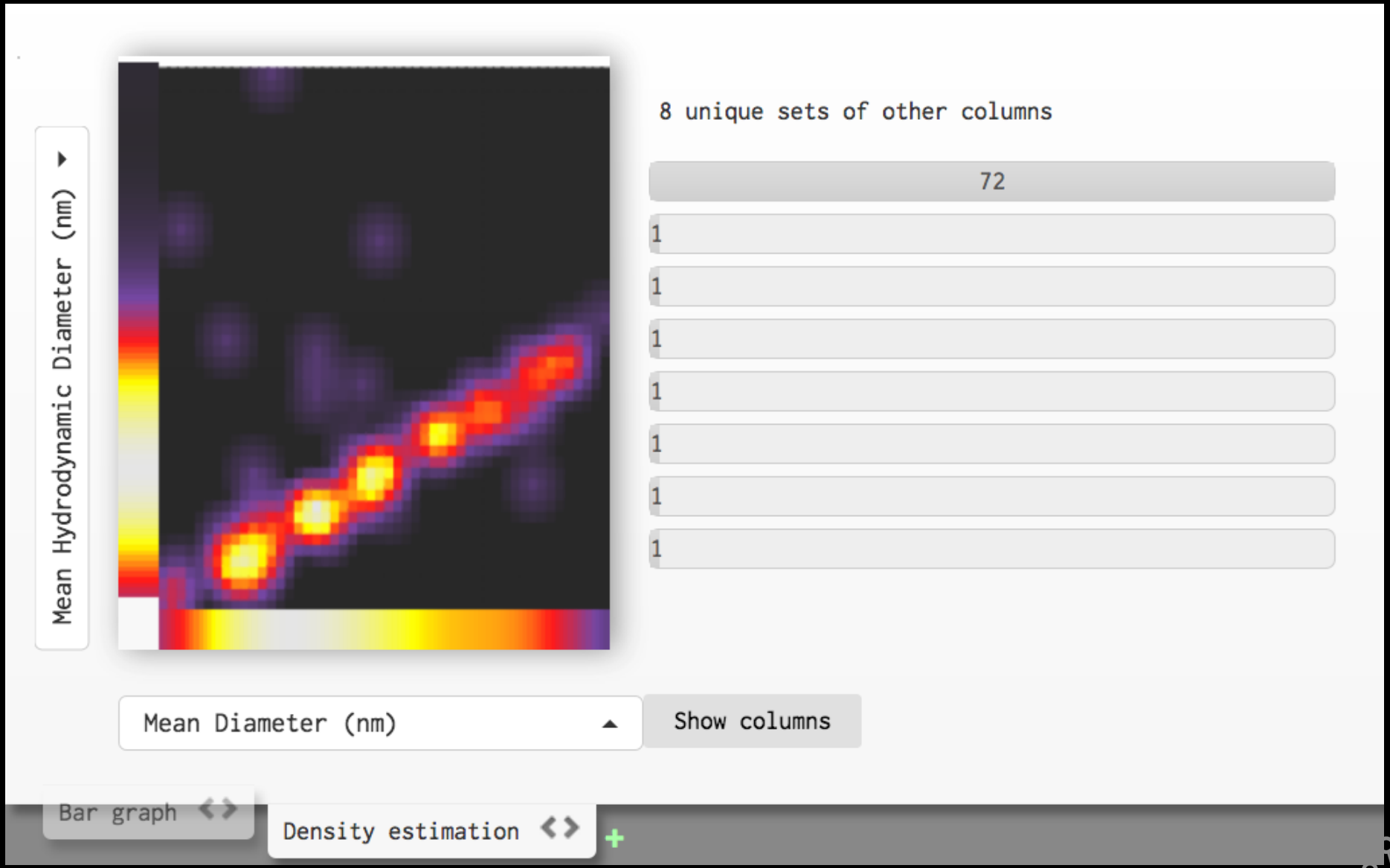


Nanomaterials registry: https://nanohub.org/resources/22014

Select the area of interest



Visualize your data

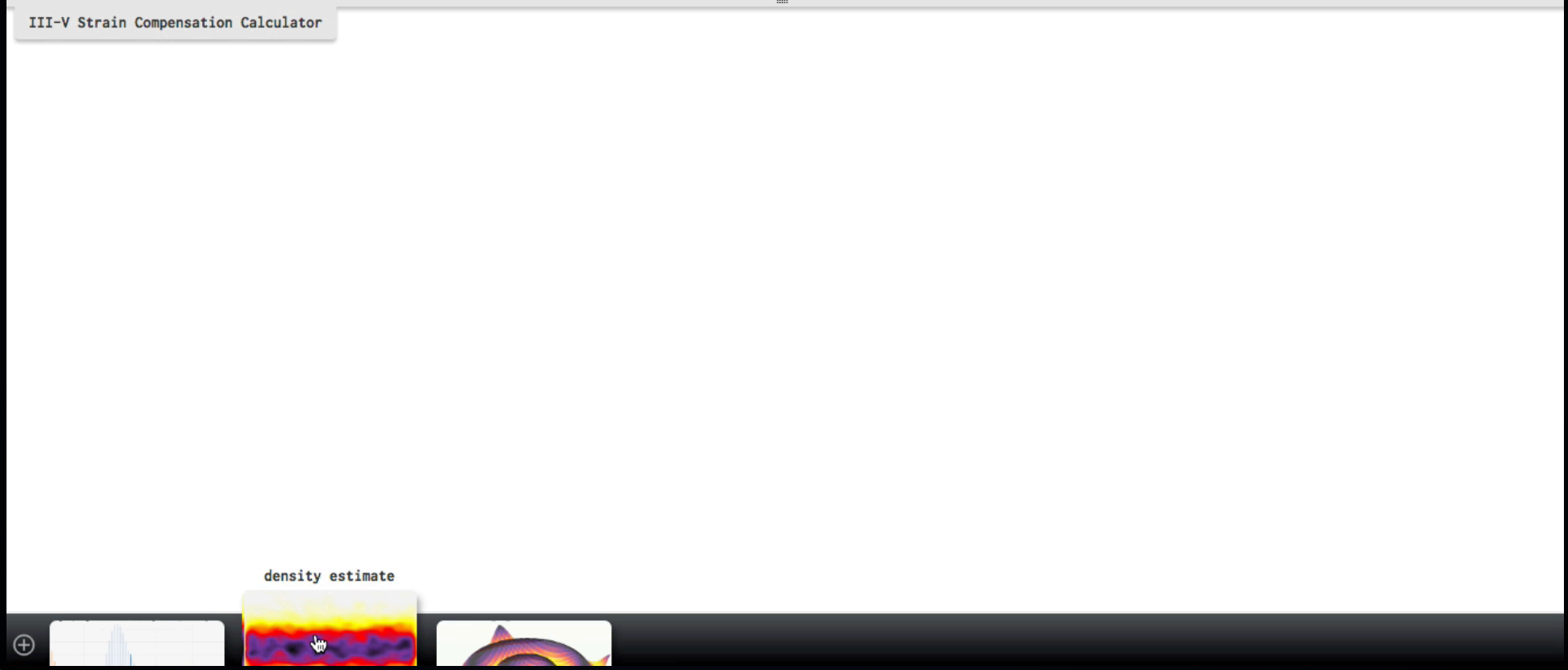


IDENT: Data Exploration & Tool Execution

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



nanoHUB

IDENT: Data Exploration & Tool Execution

Nothing selected | Use columns | Custom column | 202 total rows

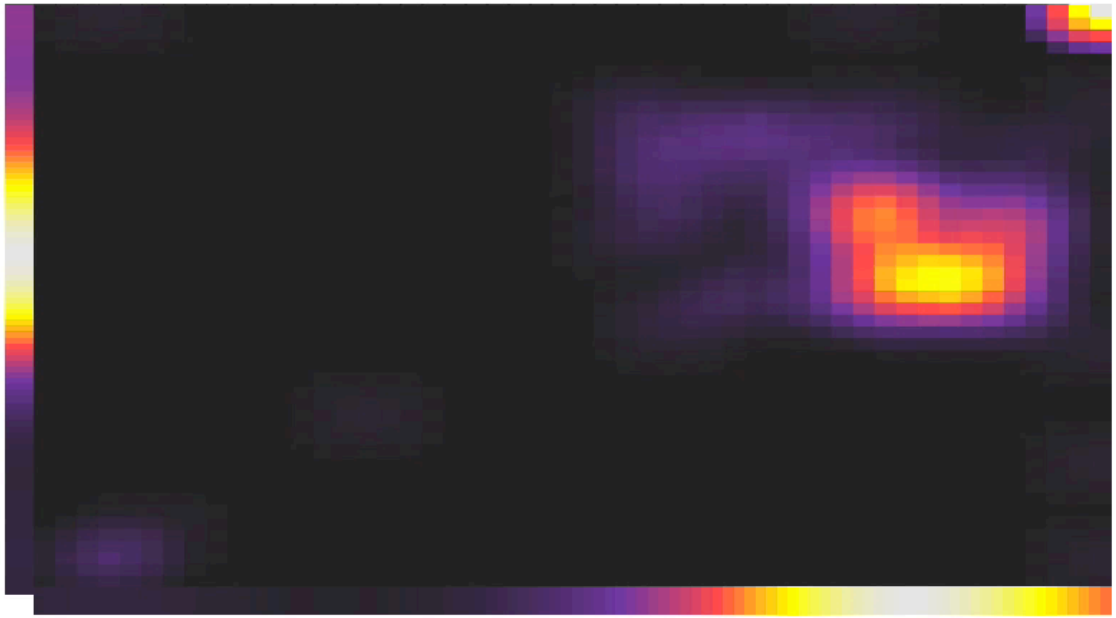
ID	Tool	Substrate x	Substrate y
1		0.7781874673773234	0.6599116204341688
2		0.833543808403423	0.746030374446
3		0.6543344226852987	0.6882546059375454
4		0.6195678131023674	0.6306212655413835
5		0.6486536880495332	0.7644257229555012
6		0.7791129291856689	0.5979152983567378
7		0.7231352091463779	0.721192957030748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

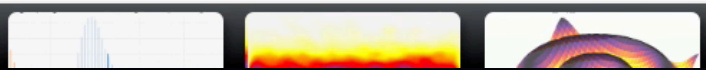
III-V Strain Compensation Calculator

X: Substrate x

Y: Substrate y

Show columns





nanoHUB

IDENT: Data Exploration & Tool Execution

Nothing selected | Use columns | Custom column | 302 total rows

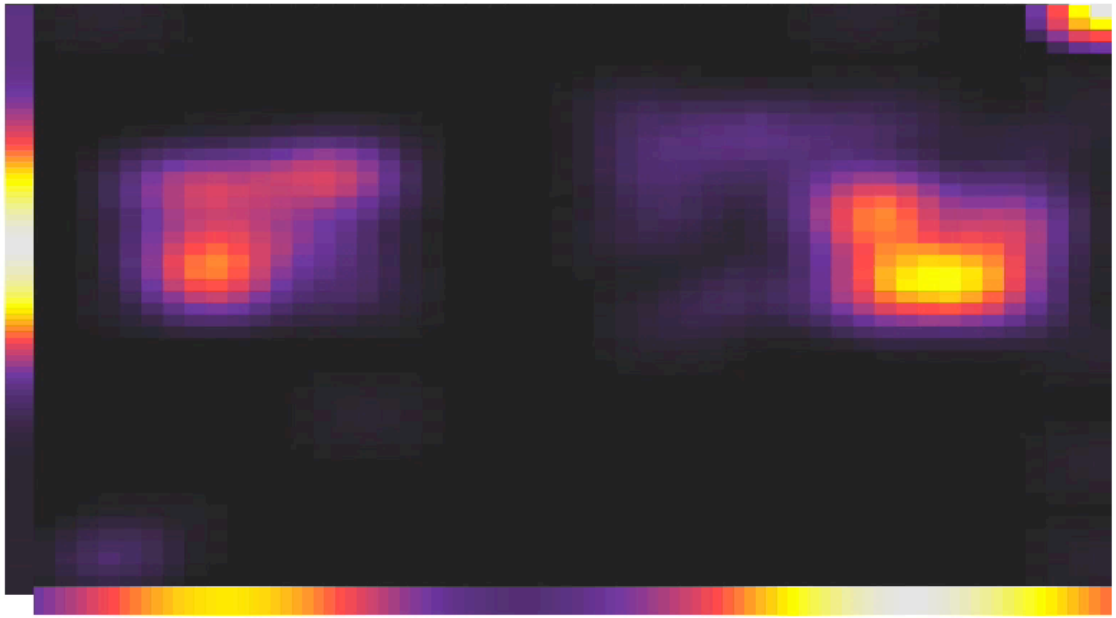
ID	Tool	Substrate x	Substrate y
1		0.7781874673773234	0.6599116204341688
2		0.833543808403423	0.746030374446
3		0.6543344226852987	0.6882546059375454
4		0.6195678131023674	0.6306212655413835
5		0.6486536880495332	0.7644257229555012
6		0.7791129291856689	0.5979152983567378
7		0.7231352091463779	0.721192957030748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

III-V Strain Compensation Calculator

X: Substrate x

Y: Substrate y

Show columns



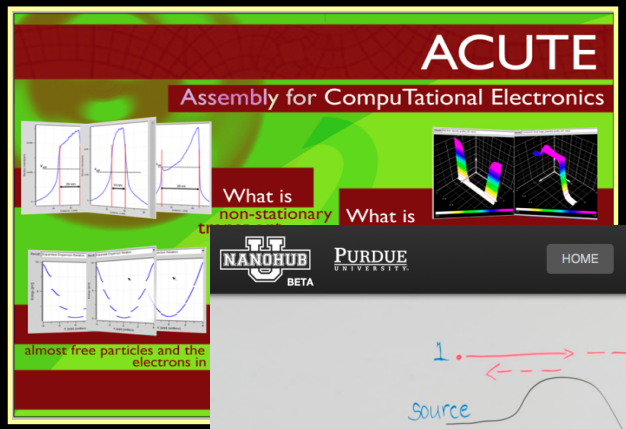
nanoHUB

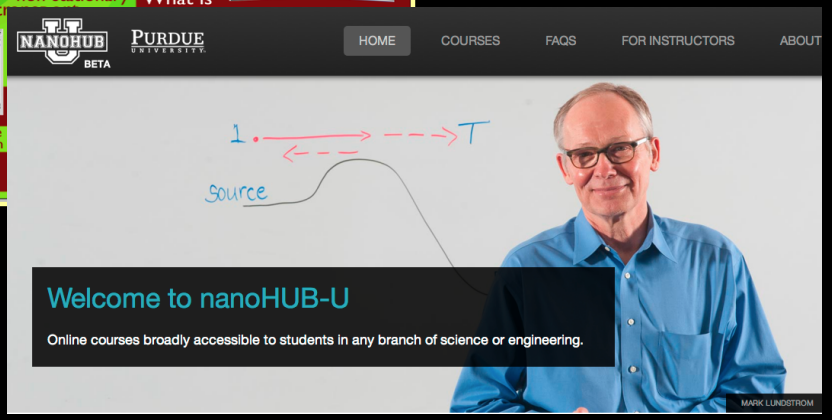
Education

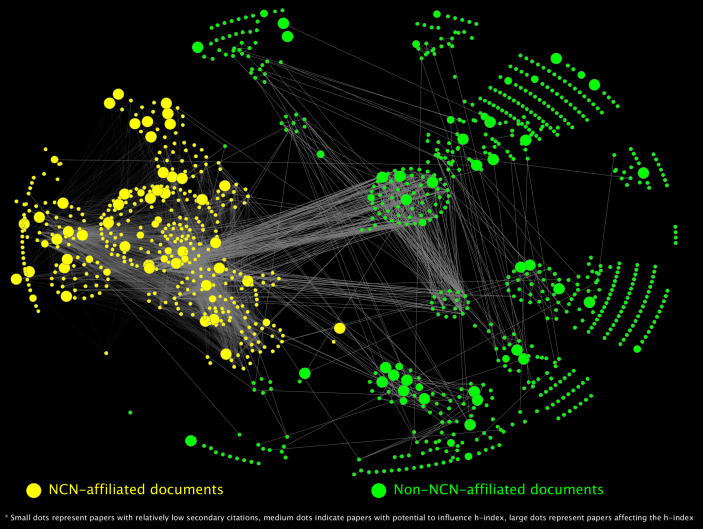
- nanoHUB-U
- 500+ teaching materials

Research in the cloud

- 400+ simulation tools
- 2,500 online seminars



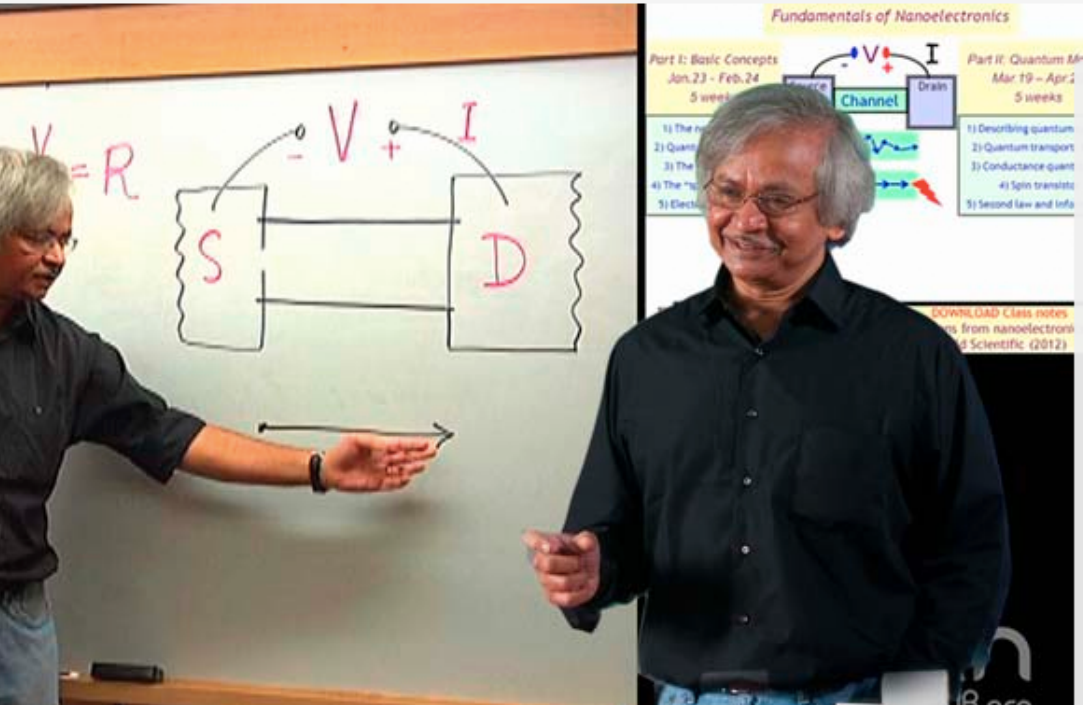




Global collaboration & community

PURDUE UNIVERSITY

"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

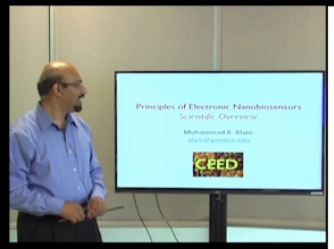
Transport Fundamentals - NEGF

nanoHUB-U courses related to materials

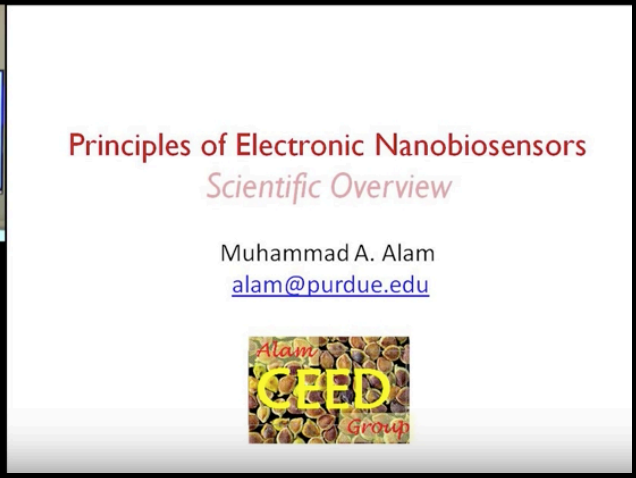
- A forum for evolving, original viewpoints that should become mainstream
- Focus on seniors, beginning grad students, working engineers
- Designed to "transcend disciplines" and be broadly accessible (no long list of prerequisites)
- Short but not too short (5 weeks) and not superficial
  - 5 20-minutes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

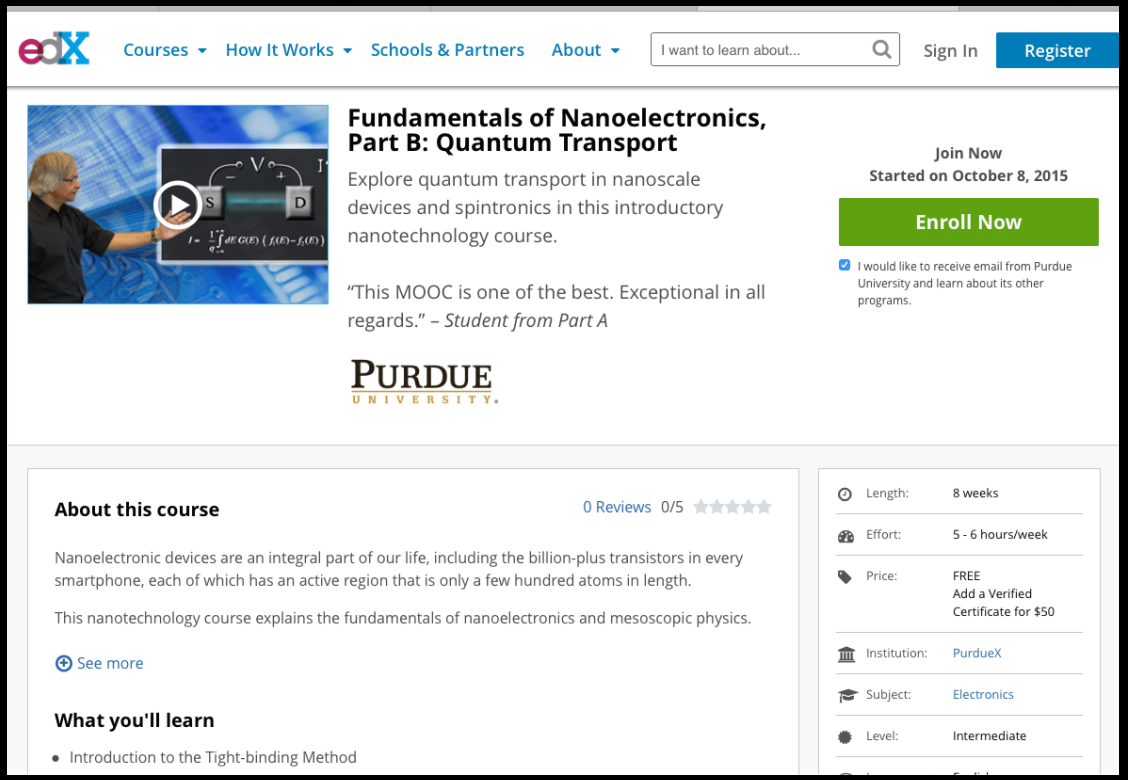
nanoHUB-U / edX in numbers

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



NANOHUB-U





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

PURDUE UNIVERSITY

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.

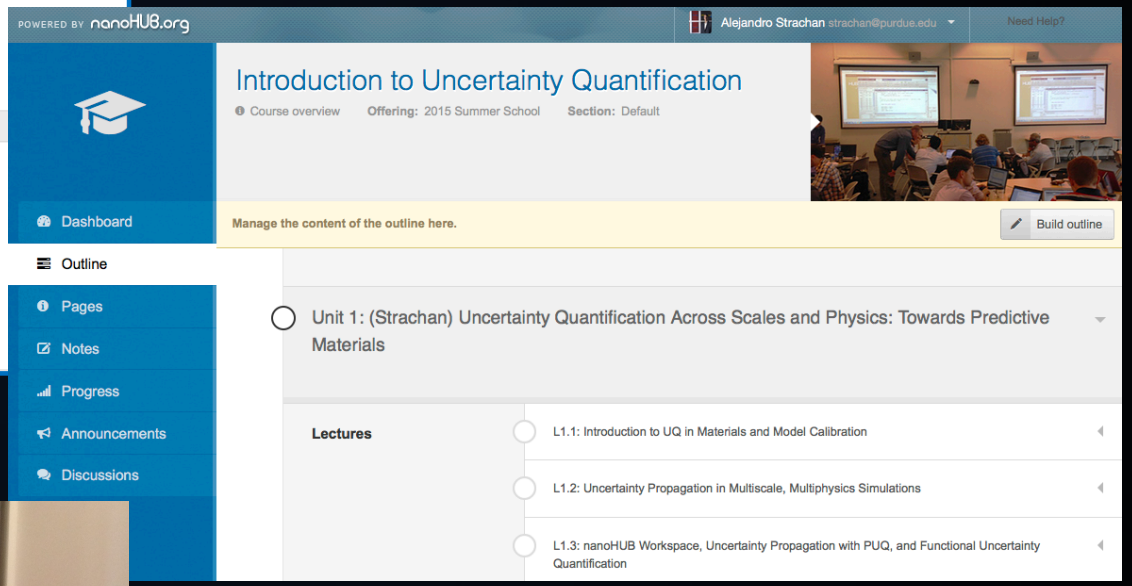
Integrity ★ Service ★ Excellence

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

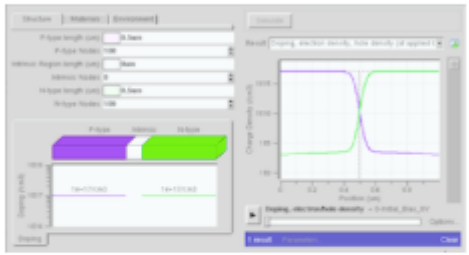


- 25% of participants from Industry: Boeing, Dow Chemical, Intel, Schrodinger, Inc., Corning Inc., Solvay Cytec

Innovate, **educate**, **engage**

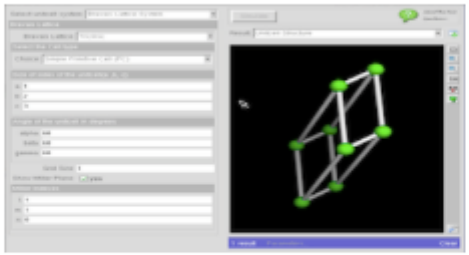
Simulation-enhanced learning

Most Popular Simulation Tools for Education



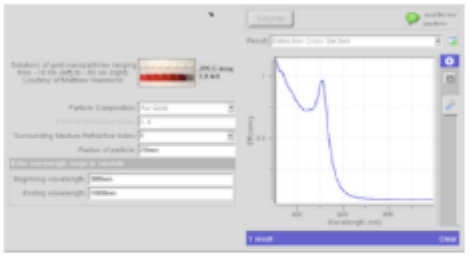
PN Junction Lab

- Launch Tool.



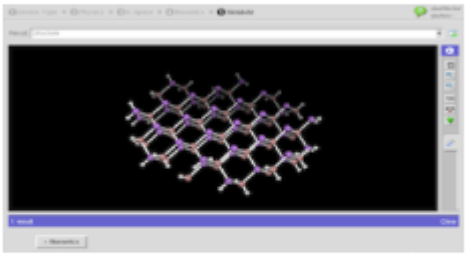
Crystal Viewer Tool

- 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

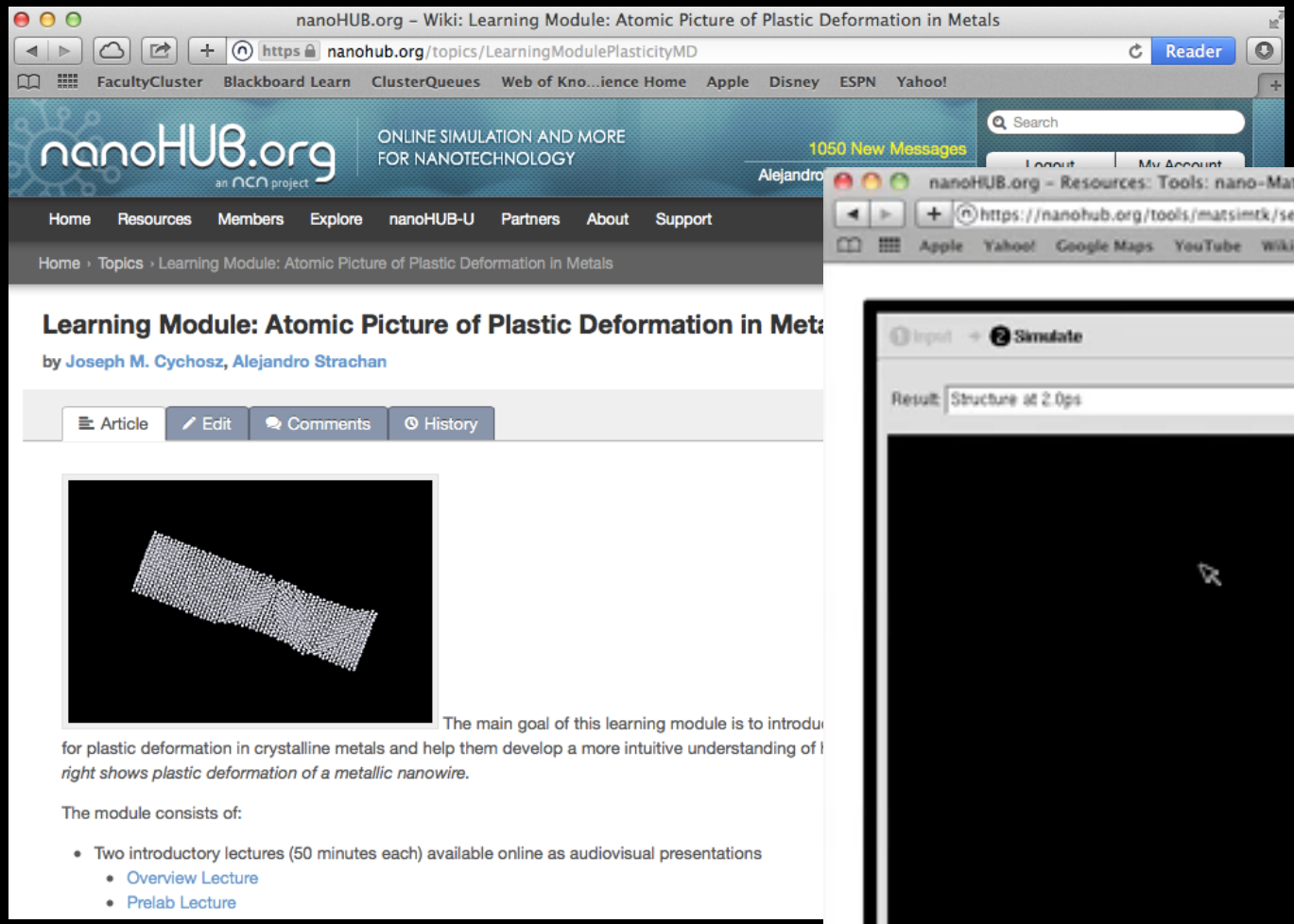
- Collection materials and overview.
- Simulation Page.

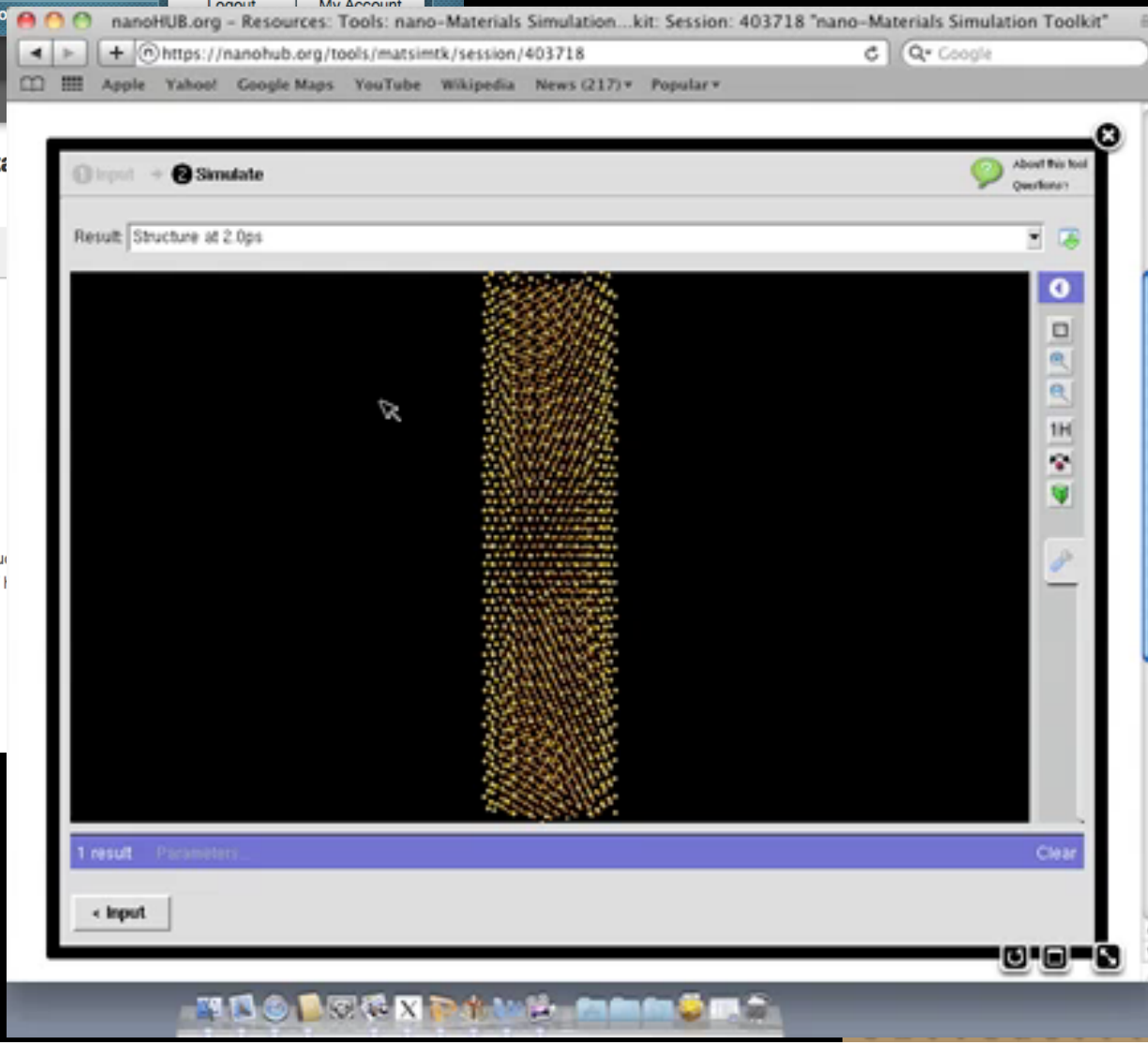
Materials Science Simulations

- Collection materials and overview.

Learning about materials using simulations

https://nanohub.org/topics/LearningModulePlasticityMD





Assessing students learning

Advances in Engineering Education

WINTER 2013

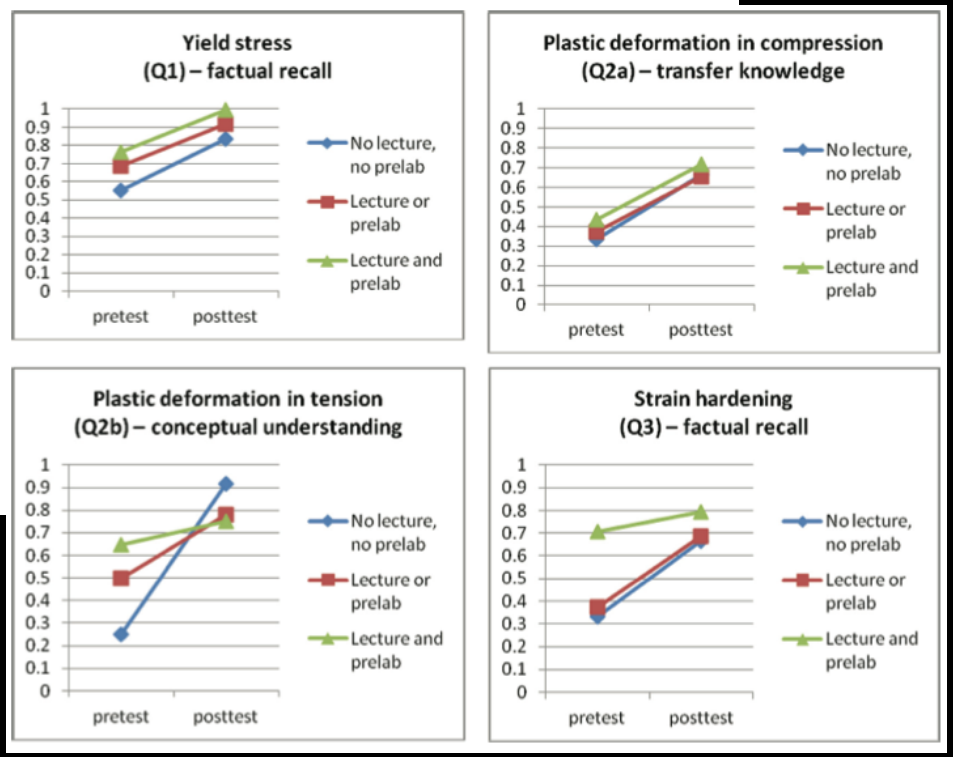
Lectures and Simulation Laboratories to Improve Learners' Conceptual Understanding

SEAN P. BROPHY
Engineering Education

ALEJANDRA J. MAGANA
Computer and Information Technology

AND

ALEJANDRO STRACHAN
Materials Engineering
Purdue University
West Lafayette, IN

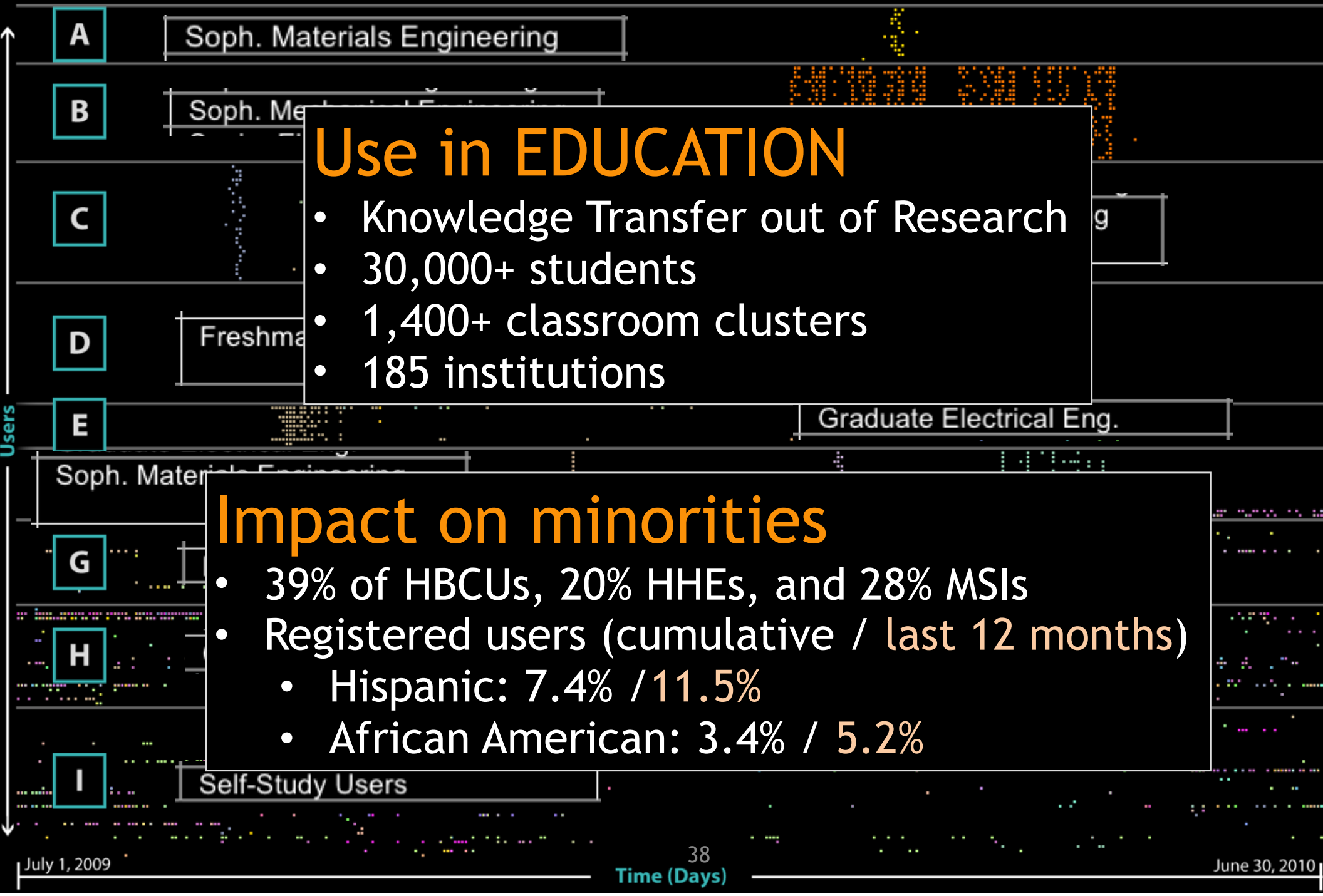


Advances in Engineering Education, 3, 1-17 (2013).

PURDUE UNIVERSITY


nanoHub User Behavior
Users
Time (days)
2010-06-30
6 users
1 days of history

nanoHUB usage statistics



Use in EDUCATION

- Knowledge Transfer out of Research
- 30,000+ students
- 1,400+ classroom clusters
- 185 institutions

Impact on minorities

- 39% of HBCUs, 20% HHEs, and 28% MSIs
- Registered users (cumulative / last 12 months)
  - Hispanic: 7.4% /11.5%
  - African American: 3.4% / 5.2%

Empowering communities

Industry

Researchers

Instructors

Students

1.4 M visitors 12,000+ simulation users per year

National Science Foundation
WHERE DISCOVERIES BEGIN

Join the materials group!

nanohub.org/groups/materials