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

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Summit on Data and Data Analytics, Evanston IL
NANO is HUGE

LARGEST NANOTECHNOLOGY ONLINE RESOURCE

400 simulation tools
1.4M visitors
4500 resources
much more than a web site
much more than a web site
much more than a web site

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

Global collaboration & community
nanoHUB

- Community driven

- NCN-cyber node develops & operates the cyberinfrastructure

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

1,600+ contributors
Tools designed for end users

Innovate, educate, engage

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
64% of papers outside NCN
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 nanomatrixushka nanoparticle (3 layer)
nanoHUB tools indexed by Web of Science

WEB OF SCIENCE™

Results: 2,251
(from All Databases)
You searched for: PUBLICATION NAME: (nanoHUB) ...More

Refine Results

Databases

Research Domains
- SCIENCE TECHNOLOGY (2,251)

Research Areas
- SCIENCE TECHNOLOGY OTHER TOPICS (2,251)

Document Types

Authors

Authors - Korean

Sort by: Relevance

Select Page

Save to EndNote online  Add to Marked List

1. NanoTCAD VIDEOS
   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 1.2.6
   Document Type: Software
   View Abstract

3. [Illinois]: Sigmoidal unit training with the delta rule
   By: Sprat, Lisa
   nanoHUB
   DOI: http://dx.doi.org/ezproxy.lib.purdue.edu/10.4231/D3S758K2N 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
- Temperature: 300K
- Temperature Gradient: 10K
- Si doping: 1e+18/cm³
- Ge doping: 1e+18/cm³
- Substrate composition SiₓGe₁₋ₓ: 1
- Mat 1 Material: Silicon
- Mat 2 Material: Germanium

Mat 1 Horizontal Thickness: 1nm
Mat 2 Horizontal Thickness: 3nm

Graph: Seebeck Coefficient vs. Mat 2 Horizontal Thickness

Simulation = #7
Mat 2 Horizontal Thickness = 3nm
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

1D Gaussian Process Regression Demo

Author
Nicos Billioudis (ibilion@purdue.edu)
PredictiveScience Lab
School of Mechanical Engineering
Purdue University, West Lafayette, IN, USA

Powered by The excellent GPy package from the University of Sheffield

variability 1.082
length_scale 1
noise_variance 0.001
optimize
plot

-x

Mean
Data
Confidence
KIM Models

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

<table>
<thead>
<tr>
<th>H</th>
<th>Li</th>
<th>Be</th>
<th>B</th>
<th>C</th>
<th>N</th>
<th>O</th>
<th>F</th>
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<tbody>
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<td>Hs</td>
<td>Mt</td>
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</table>

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.
nanoHUB tool connecting to KIM
Make a decision about your research

![Graph showing C11 (GPa), C12 (GPa), and C44 (GPa) for different materials: Angelo Moody, Mishin Mehl, Mishin, Purja Pun Mishin, Schopf AlNiCo.](openkim.org)
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

Data of interest

Visualize your data
Visualize your data
### IDENT: Data Exploration & Tool Execution

<table>
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**III-V Strain Compensation Calculator**

![density estimate](image)
IDENT: Data Exploration & Tool Execution
### Data Exploration & Tool Execution

#### Table:

<table>
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#### III-V Strain Compensation Calculator

**X:** Substrate x  
**Y:** Substrate y

[Image]
nanoHUB

Research in the cloud
• 400+ simulation tools
• 2,500 online seminars

Education
• nanoHUB-U
• 500+ teaching materials

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**!

Dr. Supriyo Datta, Professor of Electrical and Computer Engineering, Purdue University
Enroll now for the **March 25th 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)

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

- 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

- 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
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.

NCN Supported Learning Packages

nanoHUB-U

General Chemistry Simulations
- Collection materials and overview.
- Simulation Page.

ABACUS
Assembly of Basic Applications for Coordinated Understanding of Semiconductors

Materials Science Simulations
- Collection materials and overview.
Learning about materials using simulations

https://nanohub.org/topics/LearningModulePlasticityMD

Learning Module: Atomic Picture of Plastic Deformation in Metals
by Joseph M. Cychosz, Alejandro Strachan

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

The module consists of:
- Two introductory lectures (60 minutes each) available online as audiovisual presentations
  - Overview Lecture
  - Prelab Lecture
Assessing students learning

SEAN P. BROPHY
Engineering Education

ALEJANDRA J. MAGANA
Computer and Information Technology

AND

ALEJANDRO STRACHAN
Materials Engineering
Purdue University
West Lafayette, IN

WINTER 2013

Lectures and Simulation Laboratories to Improve Learners’ Conceptual Understanding

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

Simulation tools

Training & tutorial

Data

Learning materials
Join the materials group!

nanohub.org/groups/materials

Innovate, educate, engage