a PTEC project

PHARMAHUB COLLABORATION FOR PHARMACEUTICAL ENGINEERING AND SCIENCE

The NIPTE Excipients Knowledge Base
hosted by pharmaHUB

Ann Christine Catlin, Sumudinie Fernando, Sudheera Fernando

NIPTE-sponsored Conference

March 31, 2011

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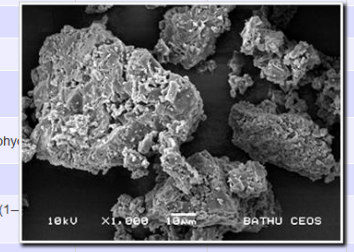
Excipients Catalog

Show 10 entries — First Previous 1 2 Next Last — Search:

ID	Compendial Name	CAS Number	Chemical Name	Description	Narrative	Image
1	α Lactose Monohydrate	5989-81-1	Lactose	-	LactoseNarrative	
2	Anhydrous α-Lactose	63-42-3	Lactose	-	LactoseNarrative	
3	Anhydrous β-Lactose	63-42-3	Lactose			
4	Microcrystalline cellulose	9004-34-6	Microcrystalline cellulose			
5	Partly Amorphous Lactose	63-42-3	Lactose			
6	Lactose Monohydrate	5989-81-1, 10039-26-6, 64044-51-5	O-β-d-Galactopyranosyl-(1→4)-α-d-glucopyranose monohyd			
7	Anhydrous Lactose	63-42-3	O-β-d-Galactopyranosyl-(1→4)-β-d-glucopyranose			
8	Lactose, Spray-Dried	5989-81-1, 10039-26-6, 64044-51-5 and 63-42-3	mixture of α-and-β-lactose, and O-β-d-galactopyranosyl-(1→ d-glucopyranose monohydrate			
9	Maltodextrin	9050-36-6	Maltodextrin	-	-	-
10	Mannitol	69-65-8	D-Mannitol	-	-	-



Excipients Database

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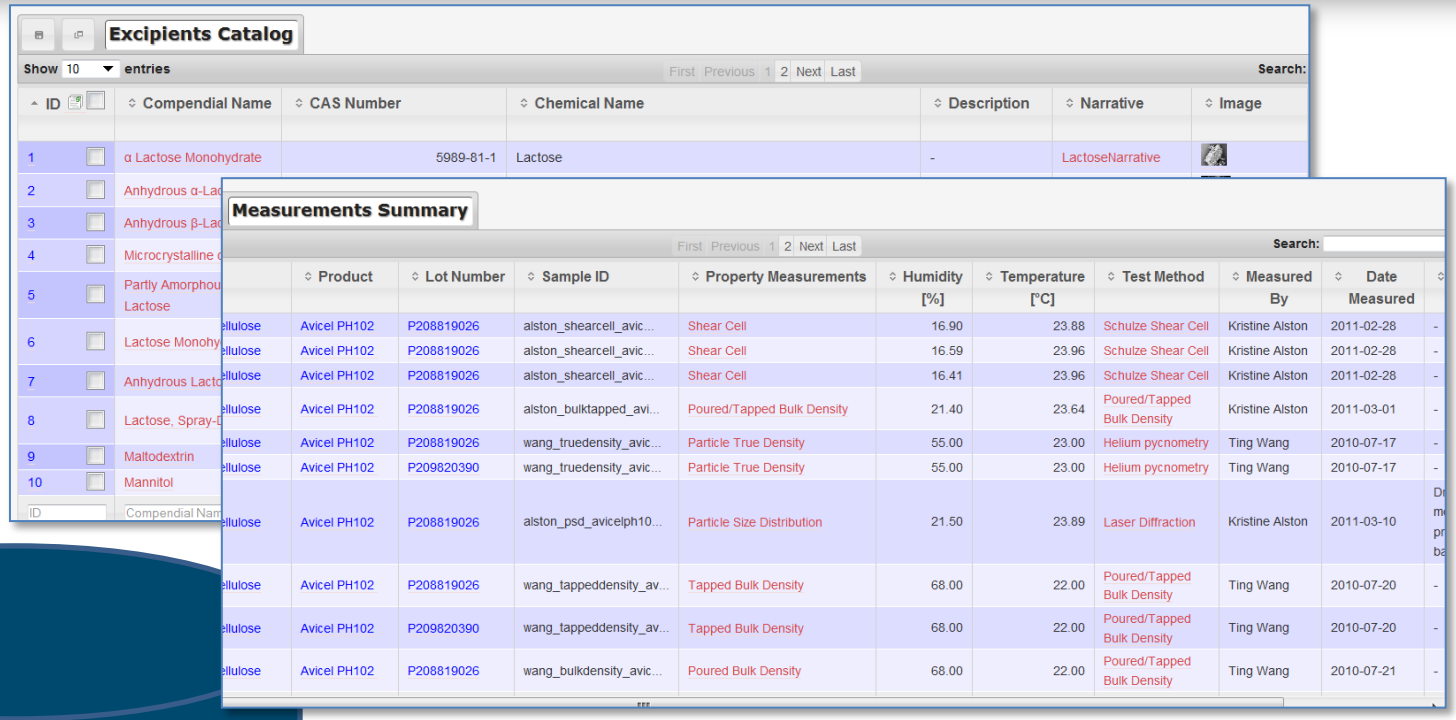

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4	Microcrystalline c					
5	Partly Amorphou Lactose					
6	Lactose Monohy					
7	Anhydrous Lacto					
8	Lactose, Spray-D					
9	Maltodextrin					
10	Mannitol					

Measurements Summary

First Previous 1 2 Next Last — Search:

	Product	Lot Number	Sample ID	Property Measurements	Humidity [%]	Temperature [°C]	Test Method	Measured By	Date Measured
llulose	Avicel PH102	P208819026	alston_shearcell_avic...	Shear Cell	16.90	23.88	Schulze Shear Cell	Kristine Alston	2011-02-28
llulose	Avicel PH102	P208819026	alston_shearcell_avic...	Shear Cell	16.59	23.96	Schulze Shear Cell	Kristine Alston	2011-02-28
llulose	Avicel PH102	P208819026	alston_shearcell_avic...	Shear Cell	16.41	23.96	Schulze Shear Cell	Kristine Alston	2011-02-28
llulose	Avicel PH102	P208819026	alston_bulktapped_avi...	Poured/Tapped Bulk Density	21.40	23.64	Poured/Tapped Bulk Density	Kristine Alston	2011-03-01
llulose	Avicel PH102	P208819026	wang_truedensity_avic...	Particle True Density	55.00	23.00	Helium pycnometry	Ting Wang	2010-07-17
llulose	Avicel PH102	P209820390	wang_truedensity_avic...	Particle True Density	55.00	23.00	Helium pycnometry	Ting Wang	2010-07-17
llulose	Avicel PH102	P208819026	alston_psd_avicelph10...	Particle Size Distribution	21.50	23.89	Laser Diffraction	Kristine Alston	2011-03-10
llulose	Avicel PH102	P208819026	wang_tappeddensity_av...	Tapped Bulk Density	68.00	22.00	Poured/Tapped Bulk Density	Ting Wang	2010-07-20
llulose	Avicel PH102	P209820390	wang_tappeddensity_av...	Tapped Bulk Density	68.00	22.00	Poured/Tapped Bulk Density	Ting Wang	2010-07-20
llulose	Avicel PH102	P208819026	wang_bulkdensity_avic...	Poured Bulk Density	68.00	22.00	Poured/Tapped Bulk Density	Ting Wang	2010-07-21

Excipients Database

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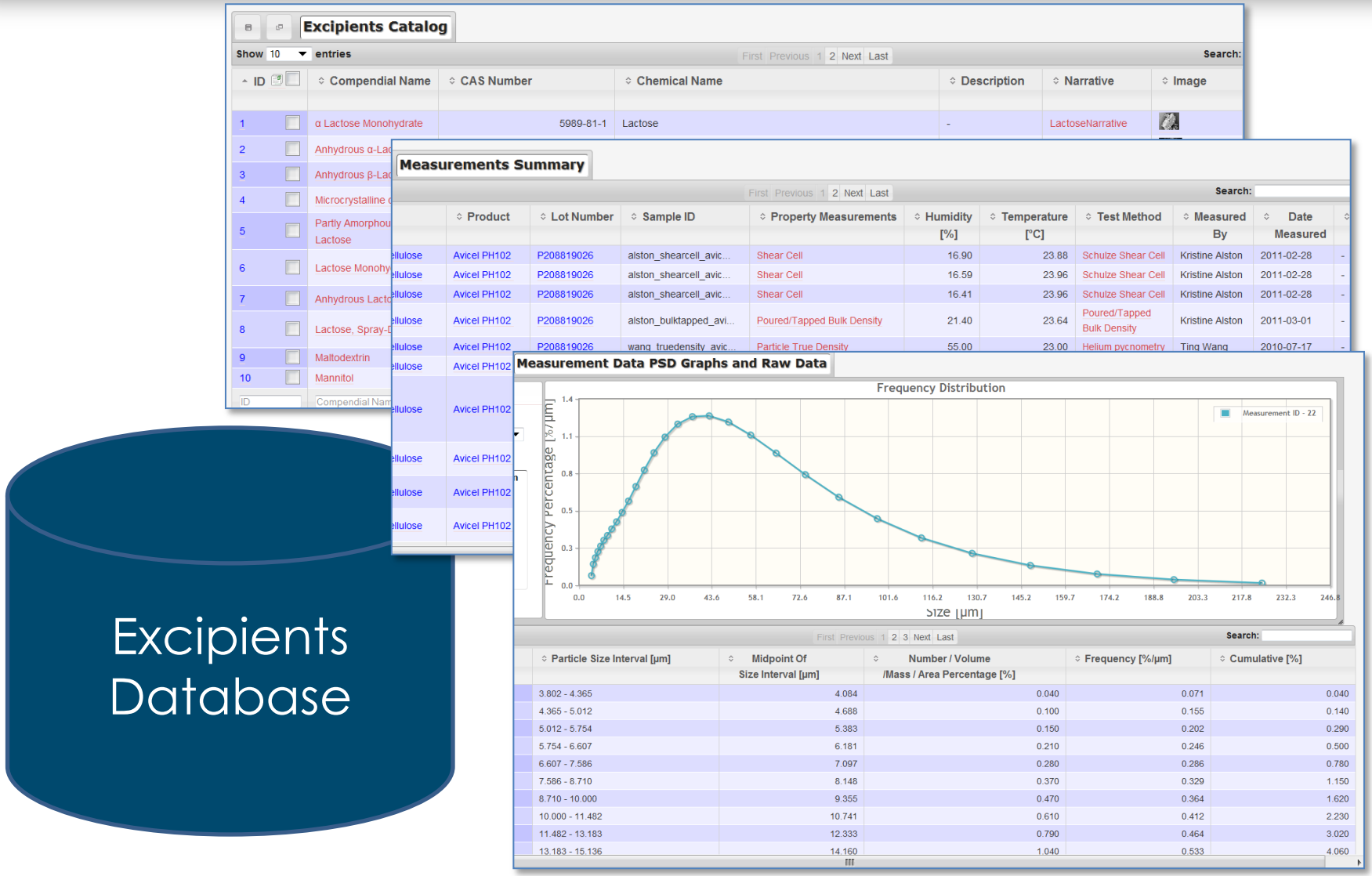
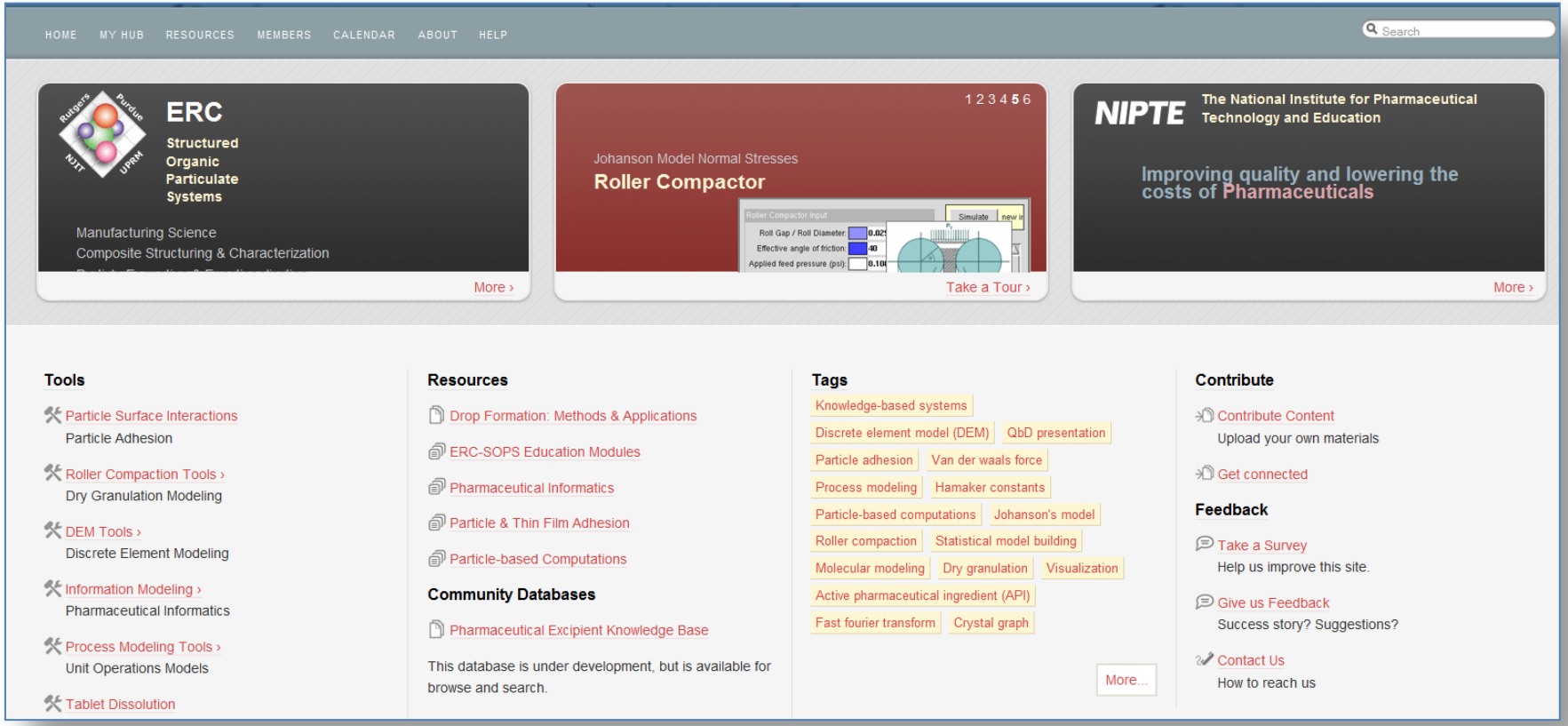


Excipients Database

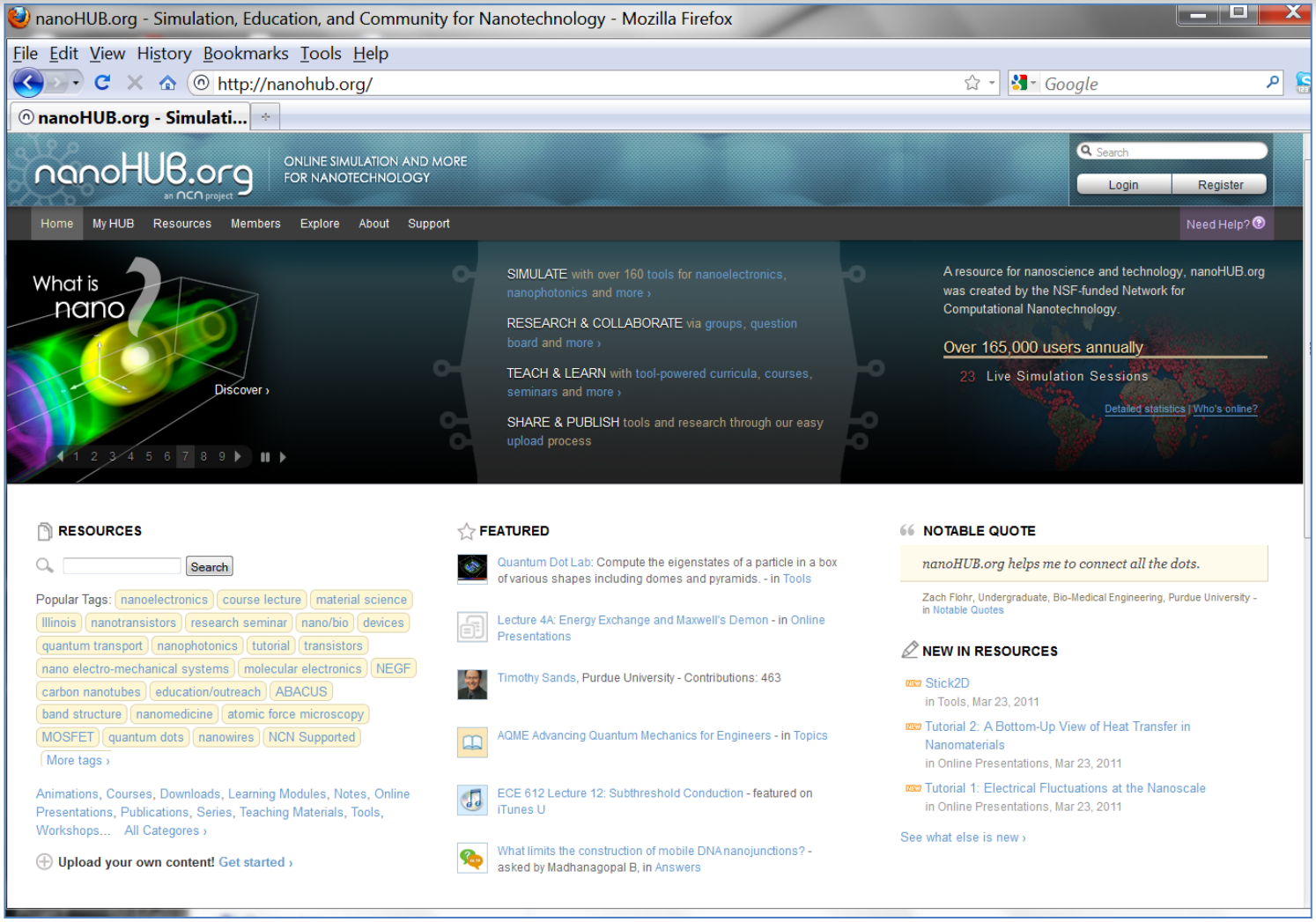
Where to Host the Database ?

pharmaHUB: a cyber infrastructure developed at Purdue University to support digital scholarship, dissemination, collaboration and outreach for the pharmaceutical engineering community.



PHARMAHUB

What is a HUB ?



nanoHUB: an environment for scientific collaboration

PHARMAHUB

Community Shared Resources

nanoHUB.org an NCN project — ONLINE SIMULATION AND MORE FOR NANOTECHNOLOGY

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You are here: Resources › Tools › Band Structure Lab › About

Band Structure Lab

By Abhijeet Paul, Mathieu Luisier, Neophytos Neophytou, Raseong Kim, Junzhe Geng, Michael McLennan, Mark Lundstrom, Gerhard Klimeck

Purdue University

Computes the electronic structure of various materials in the spatial configuration of bulk (infinitely periodic), quantum wells (confined in one dimension, infinitely periodic in 2 dimensions), and wires (confined in 2 dimensions and infinitely periodic ...

Launch Tool

Version **2.0.12** - published on 09 Dec 2010

DOI: 10254/nanohub-r1308.16 cite this

This tool is closed source.

First-Time User Guide

View All Supporting Documents

10.0 RANKING

Advanced-Expert

NCN Supported

3818 user(s), detailed usage

39 questions (Ask a question)

6 review(s) (Review this)

15 wish(es) (Add a new wish)

29 Citation(s)

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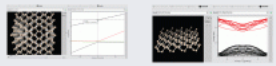

Description

Bandstructure Lab uses the *sp3s*d5* tight binding method to compute E(k) for bulk, planar, and nanowire semiconductors. Using this tool, you can quickly compute and visualize the bandstructures of bulk semiconductors, thin films, and nanowires for various materials, growth orientations, and strain conditions. Physical parameters such as the bandgap and effective mass can also be obtained from the computed E(k). The bandedges and effective masses of the bulk materials and the nanostructures structures can be analyzed as a function of various strain conditions.

As explained in a related seminar, correct band structure is essential for modeling devices at the nano scale.

- Chapter 5 of *Quantum Transport* by S. Datta (Cambridge, 2005)

SEE ALSO

- ABACUS—Introduction to Semiconductor Devices
- Part of: NCN Nanoelectronics: Simulation Tools for Education
- Part of: Quantum Mechanics: Periodic Potentials and Kronig-Penney Model
- Part of: NCN Nanoelectronics: Simulation Tools for Research
- ACUTE—Assembly for Computational Electronics
- ANTSY—Assembly for Nanotechnology Survey

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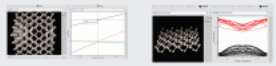

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Semiconductor Devices

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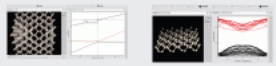

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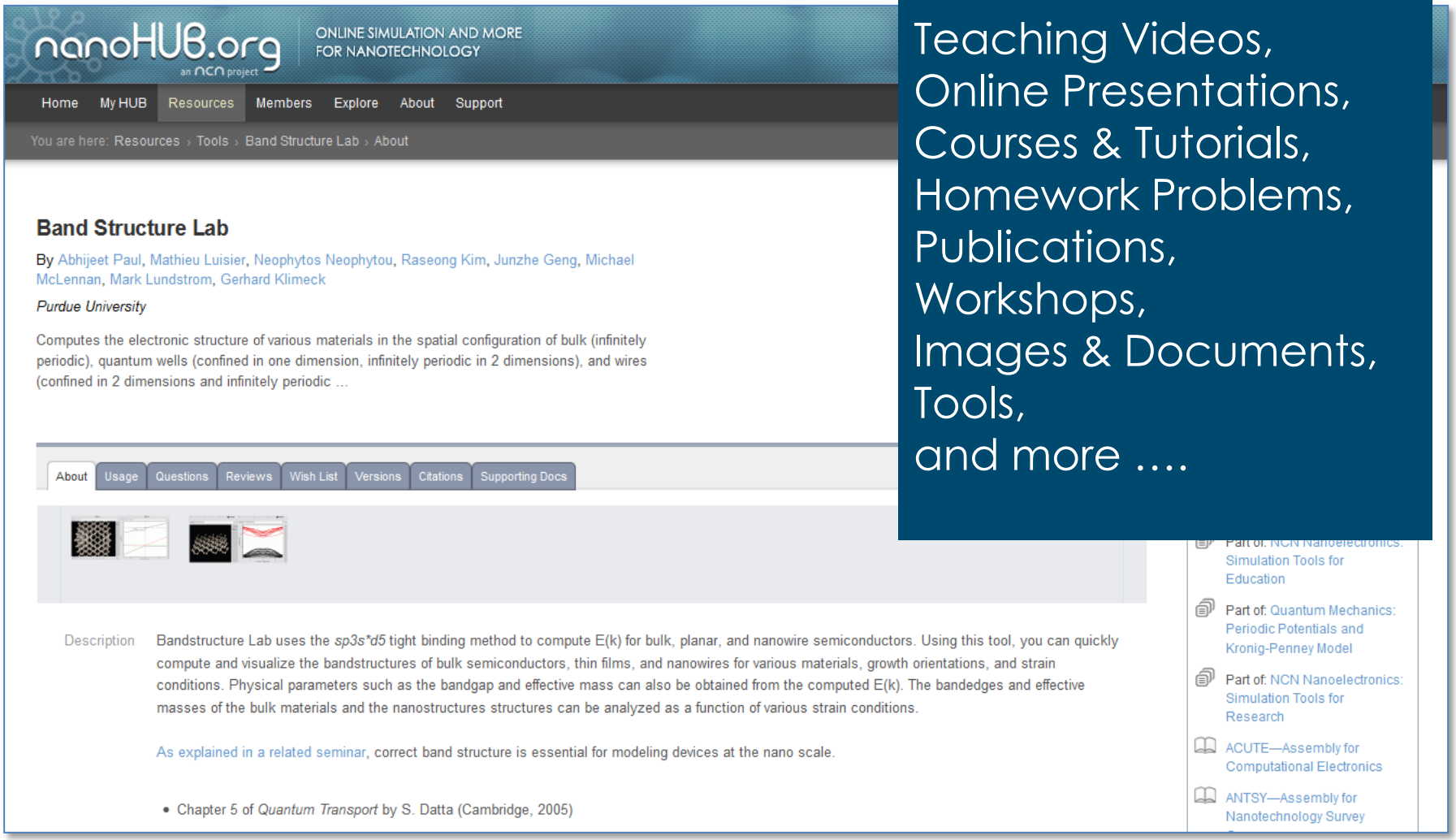
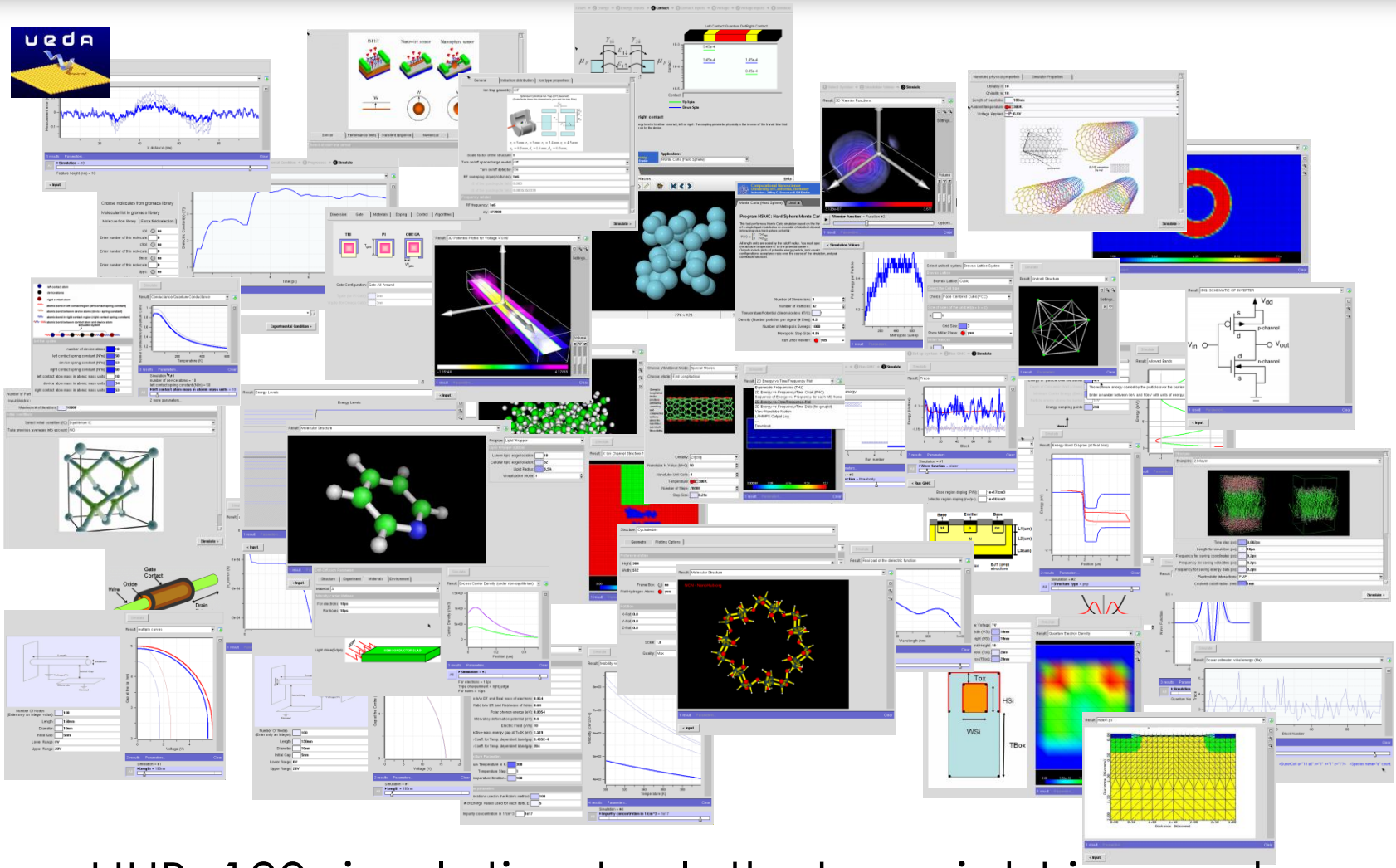


Teaching Videos,
Online Presentations,
Courses & Tutorials,
Homework Problems,
Publications,
Workshops,
Images & Documents,
Tools,
and more ….

PHARMAHUB

Simulation, Modeling, Visualization Tools

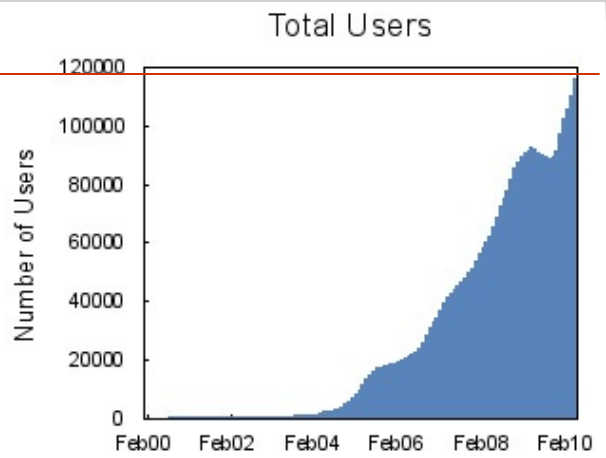


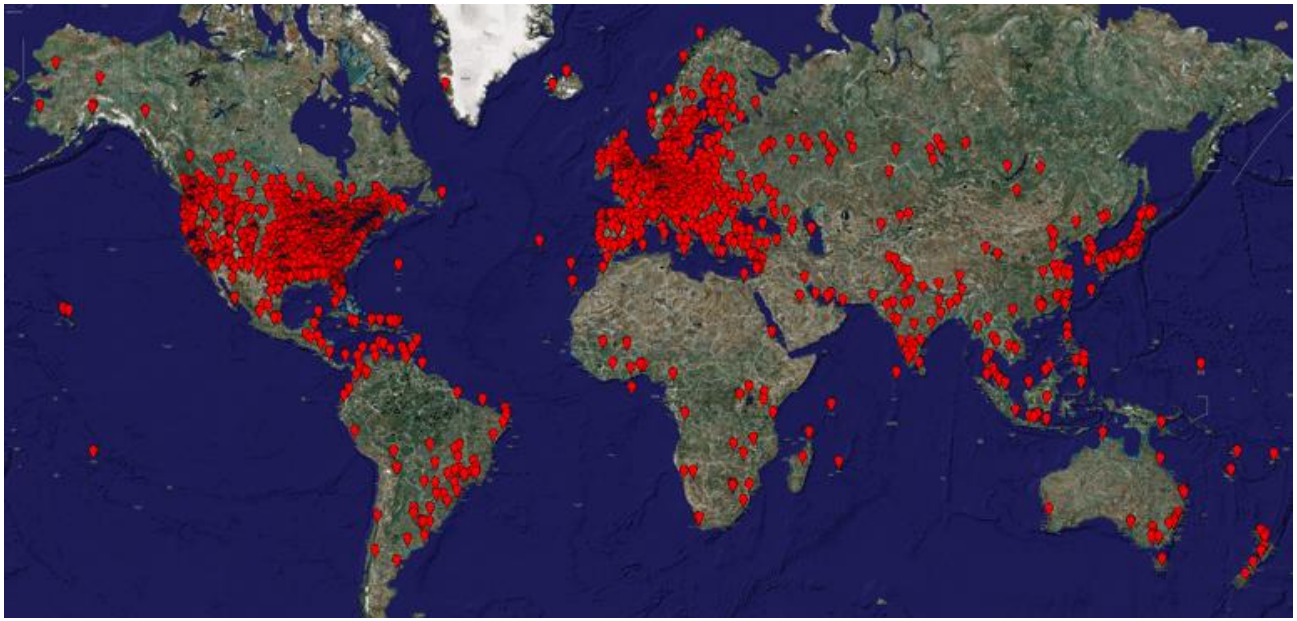
nanoHUB: 180 simulation tools that run right in your browser

Building a Scientific Community

165,000 users worldwide

>5,000,000 hits/month
Users at all top 50 US Engineering Schools
19% of all .edu domains
116 classes at 76 institutions in 2009
333 International Educational Institutions
8,200 users ran 345,000 simulations





HUBzero-powered Research Communities

- Feb 2007: 1 hub
- Feb 2008: 5 hubs
- Feb 2009: 8 hubs
- Feb 2010: 21 hubs
- Feb 2011: 30 hubs

All with their own funding streams, projects, developers

A HUB for Pharmaceutical Engineering

- Seed funding from NSF, online since December 2007
- Mission …
  - support science and engineering research in pharmaceutical manufacturing
  - offer information and decision support tools for drug product & process design
  - provide educational materials and experiences for training of pharmaceutical engineers & scientists
- More than 20,000 unique visitors in 2009-2010… with 4900 core users, 551 organizations, 105 resources and 14 simulation tools
- Ongoing funding: $1.9M NSF award to address complete product cycle development

pharmaHUB Tools

Visualization of molecular crystals
Particle-Surface Adhesion
Tablet Dissolution Model
Hopper Flow Discharge (Discrete Element Model)
Rotating Drum (DEM)
High Shear Mixer (DEM)
Continuous Particle Blending (Compartment Model)
Roller Compactor: steady state & dynamic models
Cake Filtration Model
Guideline Ontology & SWOOP Ontology Browser
Multipurpose Operation Production Planner

PHARMAHUB

pharmaHUB Courses

Statistical Model Building and Design of Experiments
Computational Methods for Molecular Crystals
Visualization of molecular crystals
Discrete Element Method (DEM)
Characterization of Nanopharmaceutical Materials
Colloids and Surfactants
Liquid Mixing Fundamentals
Sterilization and Disinfection
Mixing Equipment and Processes
API Process Unit Operations Development and Design
Pharmaceutical Bulk Drug Production

PHARMAHUB

What are the Benefits of a HUB ?

- Purdue-supported hardware and grid-computing services
- Constant support by the HUBzero Tech Team… with yearly upgrades and new technologies
- Stable and well-funded cyber infrastructure
- Contributions worldwide from academic research laboratories
- Developments from other hubs
- Database services … to build and support databases … with worldwide access

What about HUB Database Technology ?

- Contribute data with custom web-forms & spreadsheets
- Explore data with search, sort, filter, graph, compare, analyze and download
- Add images, documents, videos
- Can launch tools from data in the database
- Data catalogs : excipients, products, properties, test methods
- Measurements : interactive browsing, searching & graphing
- Community validates, rates and reviews

HUB Community: Fair & Impartial Broker

- Independent contributions from a global research community

- Pharmaceutical scientists from around the world cross-check property measurements obtained by difference methods

- Confidence in the platform, confidence in the data