



a PTEC project

COLLABORATION FOR
PHARMACEUTICAL ENGINEERING AND SCIENCE

The NIPTE Excipients Knowledge Base hosted by pharmaHUB






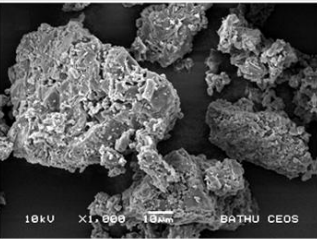





Ann Christine Catlin, Sumudinie Fernando, Sudheera Fernando
NIPTE-sponsored Conference
March 31, 2011



Excipients
Database

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 monohy		-		
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→4)-d-glucopyranose monohydrate		-		
9	Maltodextrin	9050-36-6	Maltodextrin		-	-	
10	Mannitol	69-65-8	D-Mannitol		-	-	

ID Compendial Name CAS Number Chemical Name Description Narrative Image

Excipients
Database

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	

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
Avicel PH102	P208819026	alston_shearcell_avic...	Shear Cell	16.90	23.88	Schutze Shear Cell	Kristine Alston	2011-02-28
Avicel PH102	P208819026	alston_shearcell_avic...	Shear Cell	16.59	23.96	Schutze Shear Cell	Kristine Alston	2011-02-28
Avicel PH102	P208819026	alston_shearcell_avic...	Shear Cell	16.41	23.96	Schutze Shear Cell	Kristine Alston	2011-02-28
Avicel PH102	P208819026	alston_bulktapped_avi...	Poured/Tapped Bulk Density	21.40	23.64	Poured/Tapped Bulk Density	Kristine Alston	2011-03-01
Avicel PH102	P208819026	wang_truedensity_avic...	Particle True Density	55.00	23.00	Helium pycnometry	Ting Wang	2010-07-17
Avicel PH102	P209820390	wang_truedensity_avic...	Particle True Density	55.00	23.00	Helium pycnometry	Ting Wang	2010-07-17
Avicel PH102	P208819026	alston_psd_aviceph10...	Particle Size Distribution	21.50	23.89	Laser Diffraction	Kristine Alston	2011-03-10
Avicel PH102	P208819026	wang_tappeddensity_av...	Tapped Bulk Density	68.00	22.00	Poured/Tapped Bulk Density	Ting Wang	2010-07-20
Avicel PH102	P209820390	wang_tappeddensity_av...	Tapped Bulk Density	68.00	22.00	Poured/Tapped Bulk Density	Ting Wang	2010-07-20
Avicel PH102	P208819026	wang_bulkdensity_avic...	Poured Bulk Density	68.00	22.00	Poured/Tapped Bulk Density	Ting Wang	2010-07-21

Excipients Database

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-Lac										
3	Anhydrous β-Lac										
4	Microcrystalline										
5	Partly Amorphous Lactose										
6	Lactose Monohydrate	Avicel PH102	P208819026	alston_shearcell_avi...	Shear Cell	16.90	23.88	Schutze Shear Cell	Kristine Alston	2011-02-28	-
7	Anhydrous Lactose	Avicel PH102	P208819026	alston_shearcell_avi...	Shear Cell	16.59	23.96	Schutze Shear Cell	Kristine Alston	2011-02-28	-
8	Lactose, Spray-D	Avicel PH102	P208819026	alston_bulkapped_avi...	Poured/Tapped Bulk Density	21.40	23.64	Poured/Tapped Bulk Density	Kristine Alston	2011-03-01	-
9	Maltodextrin	Avicel PH102	P208819026	wang_truedensity_avi...	Particle True Density	55.00	23.00	Helium pycnometry	Ting Wang	2010-07-17	-
10	Mannitol	Avicel PH102									

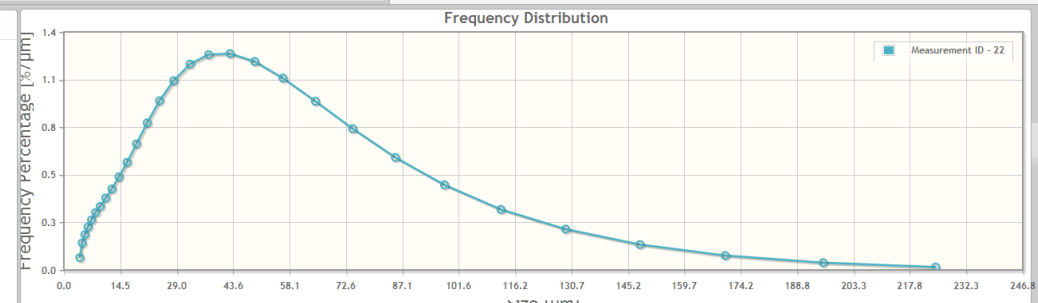
Measurements Summary

First Previous 1 2 Next Last Search:

Product	Lot Number	Sample ID	Property Measurements	Humidity [%]	Temperature [°C]	Test Method	Measured By	Date Measured
Avicel PH102	P208819026	alston_shearcell_avi...	Shear Cell	16.90	23.88	Schutze Shear Cell	Kristine Alston	2011-02-28
Avicel PH102	P208819026	alston_shearcell_avi...	Shear Cell	16.59	23.96	Schutze Shear Cell	Kristine Alston	2011-02-28
Avicel PH102	P208819026	alston_shearcell_avi...	Shear Cell	16.41	23.96	Schutze Shear Cell	Kristine Alston	2011-02-28
Avicel PH102	P208819026	alston_bulkapped_avi...	Poured/Tapped Bulk Density	21.40	23.64	Poured/Tapped Bulk Density	Kristine Alston	2011-03-01
Avicel PH102	P208819026	wang_truedensity_avi...	Particle True Density	55.00	23.00	Helium pycnometry	Ting Wang	2010-07-17

Measurement Data PSD Graphs and Raw Data

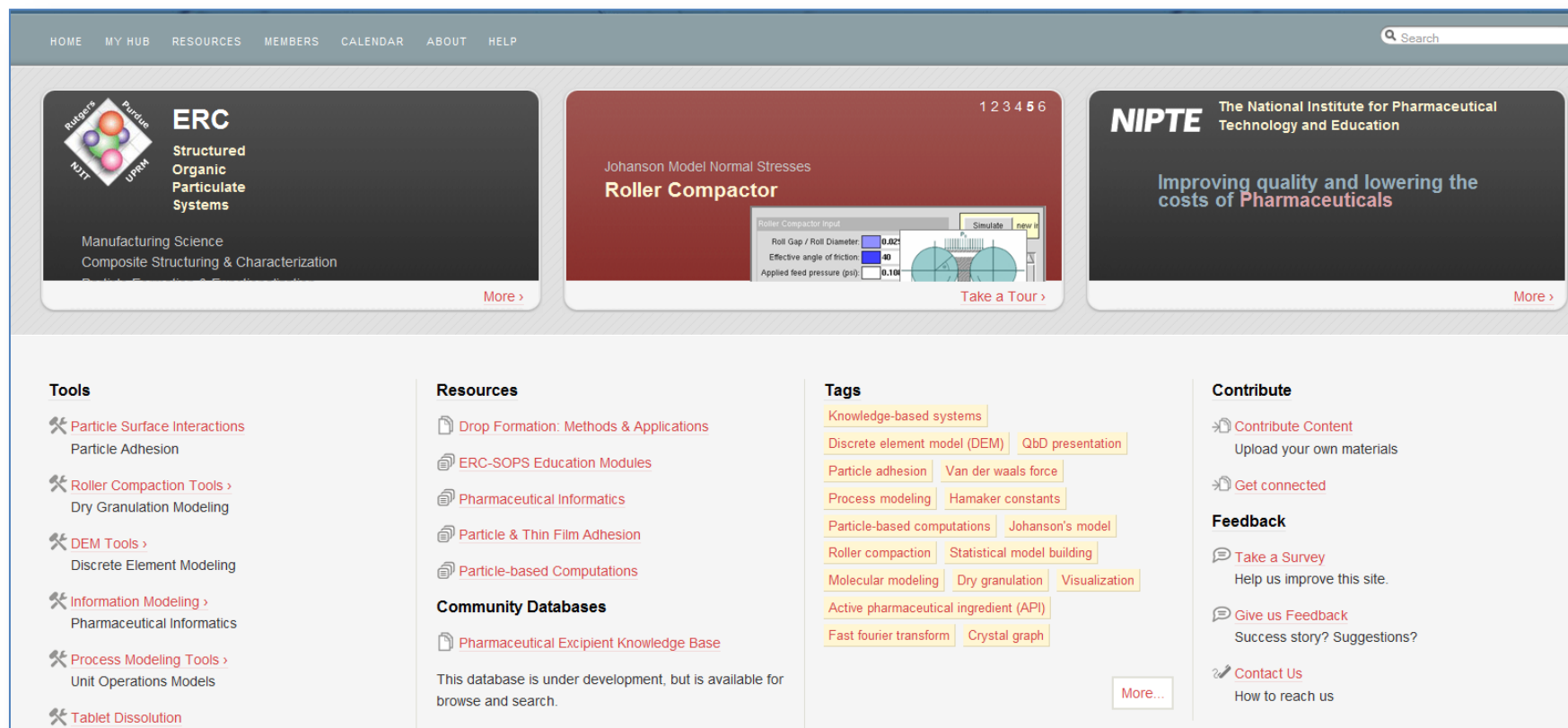
Frequency Distribution



Particle Size Interval [μm]	Midpoint Of Size Interval [μm]	Number / Volume / Mass / Area Percentage [%]	Frequency [%/μm]	Cumulative [%]
3.802 - 4.365	4.084	0.040	0.071	0.040
4.365 - 5.012	4.688	0.100	0.155	0.140
5.012 - 5.754	5.383	0.150	0.202	0.290
5.754 - 6.607	6.181	0.210	0.246	0.500
6.607 - 7.586	7.097	0.280	0.286	0.780
7.586 - 8.710	8.148	0.370	0.329	1.150
8.710 - 10.000	9.355	0.470	0.364	1.620
10.000 - 11.482	10.741	0.610	0.412	2.230
11.482 - 13.183	12.333	0.790	0.464	3.020
13.183 - 15.136	14.160	1.040	0.533	4.060

Excipients Database

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

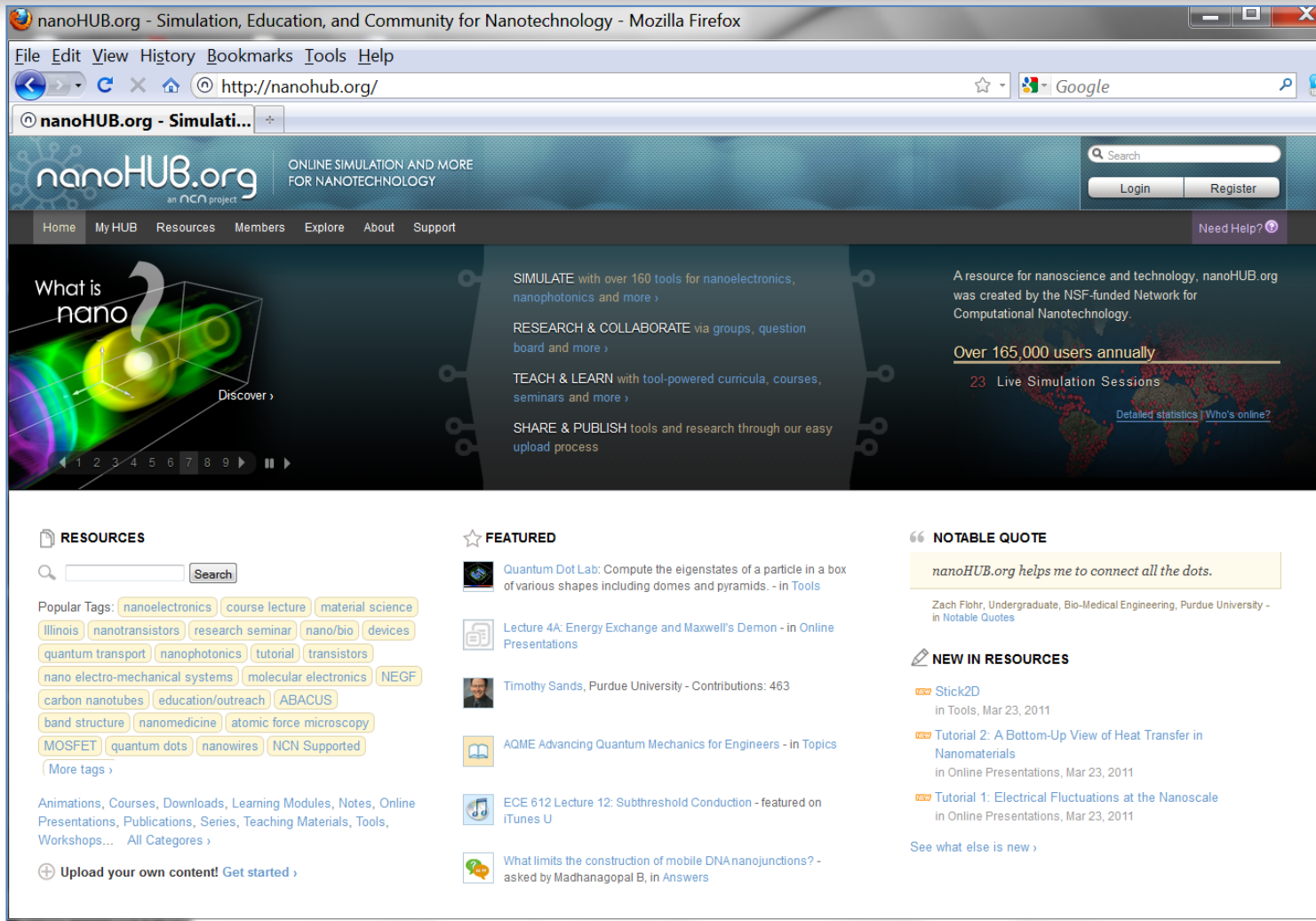


The screenshot shows the pharmaHUB website interface. At the top, there is a navigation bar with links for HOME, MY HUB, RESOURCES, MEMBERS, CALENDAR, ABOUT, and HELP, along with a search bar. Below the navigation bar, there are three main featured sections:

- ERC (Structured Organic Particulate Systems):** A dark-themed box with a logo showing a molecule and pills. Text includes "Manufacturing Science" and "Composite Structuring & Characterization". A "More >" link is at the bottom right.
- Johanson Model Normal Stresses Roller Compactor:** A red-themed box featuring a simulation interface for a roller compactor. Parameters shown include Roll Gap / Roll Diameter (0.02), Effective angle of friction (40), and Applied feed pressure (psi) (0.10). A "Take a Tour >" link is at the bottom right.
- NIPTE (The National Institute for Pharmaceutical Technology and Education):** A dark-themed box with the tagline "Improving quality and lowering the costs of Pharmaceuticals". A "More >" link is at the bottom right.

Below these featured sections, the website is organized into four columns:

- Tools:** Lists various tools such as Particle Surface Interactions, Roller Compaction Tools, DEM Tools, Information Modeling, Process Modeling Tools, and Tablet Dissolution.
- Resources:** Lists educational and informational resources like Drop Formation: Methods & Applications, ERC-SOPS Education Modules, Pharmaceutical Informatics, Particle & Thin Film Adhesion, Particle-based Computations, and Pharmaceutical Excipient Knowledge Base. It also includes a note: "This database is under development, but is available for browse and search." and a "More..." link.
- Tags:** A collection of yellow tags representing different topics, including Knowledge-based systems, Discrete element model (DEM), QbD presentation, Particle adhesion, Van der waals force, Process modeling, Hamaker constants, Particle-based computations, Johanson's model, Roller compaction, Statistical model building, Molecular modeling, Dry granulation, Visualization, Active pharmaceutical ingredient (API), Fast fourier transform, and Crystal graph.
- Contribute:** Encourages user participation with options like "Contribute Content" (Upload your own materials), "Get connected", "Feedback" (Take a Survey, Give us Feedback, Contact Us), and "Success story? Suggestions?".



The screenshot shows the nanoHUB.org website interface. At the top, the browser title is "nanoHUB.org - Simulation, Education, and Community for Nanotechnology - Mozilla Firefox". The address bar shows "http://nanohub.org/". The website header includes the nanoHUB.org logo, the tagline "ONLINE SIMULATION AND MORE FOR NANOTECHNOLOGY", and a search bar with "Login" and "Register" buttons. A navigation menu contains "Home", "My HUB", "Resources", "Members", "Explore", "About", and "Support".

The main content area features a large video player on the left with the text "What is nano?" and a "Discover" button. To the right, there are three columns of text:

- SIMULATE** with over 160 tools for nanoelectronics, nanophotonics and more >
- RESEARCH & COLLABORATE** via groups, question board and more >
- TEACH & LEARN** with tool-powered curricula, courses, seminars and more >
- SHARE & PUBLISH** tools and research through our easy upload process

On the right side of the main content, there is a summary box: "A resource for nanoscience and technology, nanoHUB.org was created by the NSF-funded Network for Computational Nanotechnology." Below this, it states "Over 165,000 users annually" and "23 Live Simulation Sessions" with links for "Detailed statistics" and "Who's online?".

The bottom section is divided into three columns:

- RESOURCES**: Includes a search bar and a list of popular tags such as "nanoelectronics", "course lecture", "material science", "illinois", "nanotransistors", "research seminar", "nano/bio", "devices", "quantum transport", "nanophotonics", "tutorial", "transistors", "nano electro-mechanical systems", "molecular electronics", "NEGF", "carbon nanotubes", "education/outreach", "ABACUS", "band structure", "nanomedicine", "atomic force microscopy", "MOSFET", "quantum dots", "nanowires", and "NCN Supported". A "More tags >" link is also present.
- FEATURED**: Lists featured content including "Quantum Dot Lab: Compute the eigenstates of a particle in a box of various shapes including domes and pyramids. - in Tools", "Lecture 4A: Energy Exchange and Maxwell's Demon - in Online Presentations", "Timothy Sands, Purdue University - Contributions: 463", "AQME Advancing Quantum Mechanics for Engineers - in Topics", "ECE 612 Lecture 12: Subthreshold Conduction - featured on iTunes U", and "What limits the construction of mobile DNA nanojunctions? - asked by Madhanagopal B, in Answers".
- NOTABLE QUOTE**: A quote from Zach Flehr, Undergraduate, Bio-Medical Engineering, Purdue University: "nanoHUB.org helps me to connect all the dots." Below the quote is a link to "Notable Quotes".
- NEW IN RESOURCES**: Lists recent additions like "Stick2D in Tools, Mar 23, 2011", "Tutorial 2: A Bottom-Up View of Heat Transfer in Nanomaterials in Online Presentations, Mar 23, 2011", and "Tutorial 1: Electrical Fluctuations at the Nanoscale in Online Presentations, Mar 23, 2011". A "See what else is new >" link is provided.

At the bottom left, there is a link to "Upload your own content! Get started >".

nanoHUB: an environment for scientific collaboration

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)

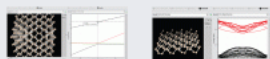
 6 review(s) (Review this)

 15 wish(es) (Add a new wish)

 29 Citation(s)

Share: 

[About](#) [Usage](#) [Questions](#) [Reviews](#) [Wish List](#) [Versions](#) [Citations](#) [Supporting Docs](#)









Description Bandstructure Lab uses the $sp^3s^*d^5$ 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](#)
-  [ANTSYS—Assembly for Nanotechnology Survey](#)

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

Home My HUB Resources Members Explore About Support

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

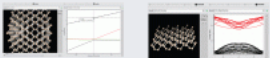
Band Structure Lab

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 ...)

About Usage Questions Reviews Wish List Versions Citations Supporting Docs



Description Bandstructure Lab uses the $sp^3s^*d^5$ 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)

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)

Share:    ...

- 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
 - ANTSYS—Assembly for Nanotechnology Survey

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 ...

About Usage Questions Reviews Wish List Versions Citations Supporting Docs



Description Bandstructure Lab uses the $sp^3s^*d^5$ 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)

Search Tags,
Found by Google,
Recommendations,
“See Also”

CC BY-NC-ND 4.0 International license


This tool is closed source.

 [First-Time User Guide](#)

[View All Supporting Documents](#)

 39 questions ([Ask a question](#))


 6 review(s) ([Review this](#))

 15 wish(es) ([Add a new wish](#))


 29 Citation(s)

Share:     ...

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](#)

 [ANTSYS—Assembly for Nanotechnology Survey](#)

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 ...)

About Usage Questions Reviews Wish List Versions Citations Supporting Docs



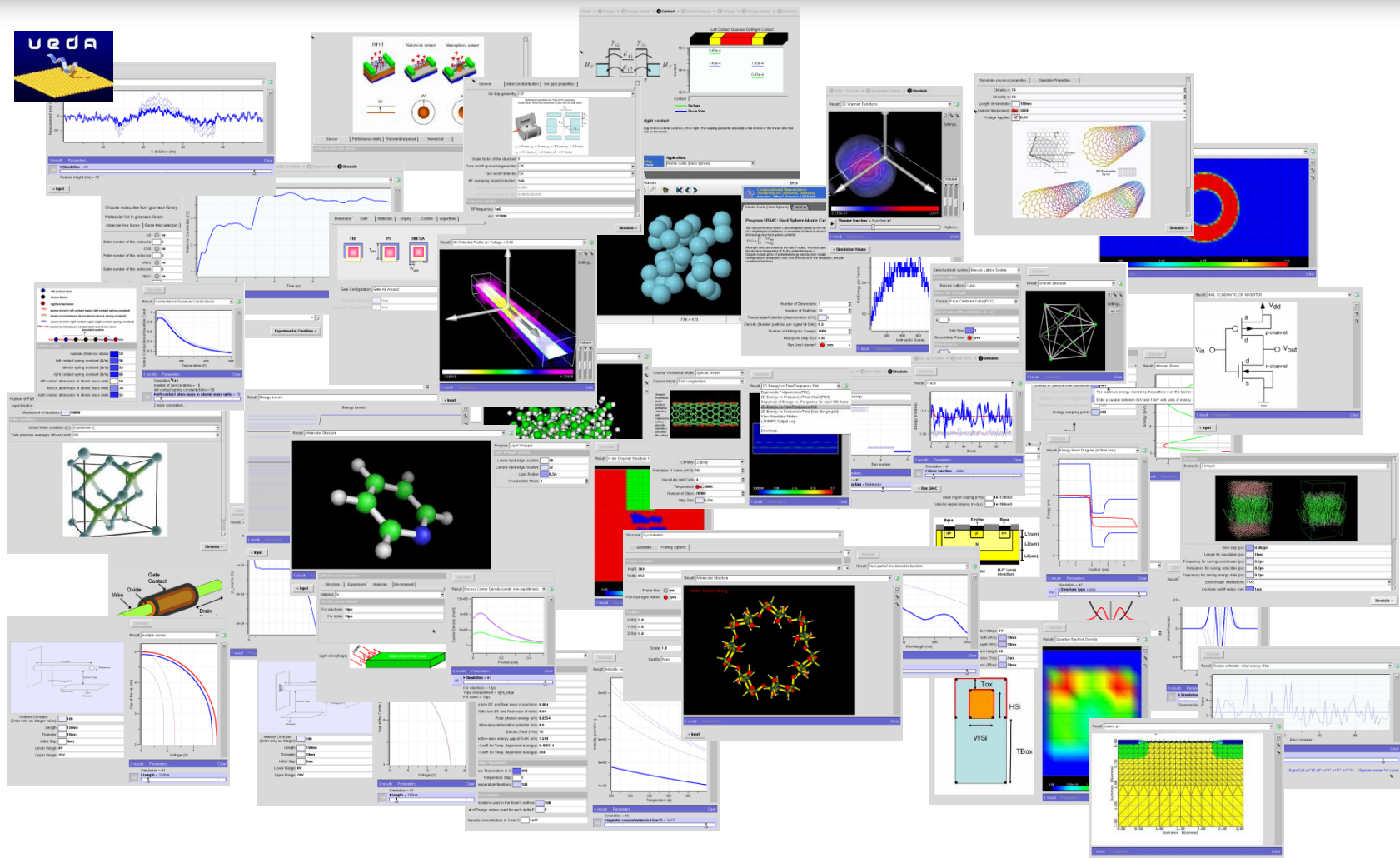
Description Bandstructure Lab uses the $sp^3s^*d^5$ tight binding method to compute $E(k)$ for bulk, planar, and nanowire semiconductors. Using this tool, you can quickly compute and visualize the bandstructures of bulk semiconductors, thin films, and nanowires for various materials, growth orientations, 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)

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

- 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
- ANTS—Assembly for Nanotechnology Survey



nanoHUB: 180 simulation tools that run right in your browser

165,000 users worldwide

>5,000,000 hits/month

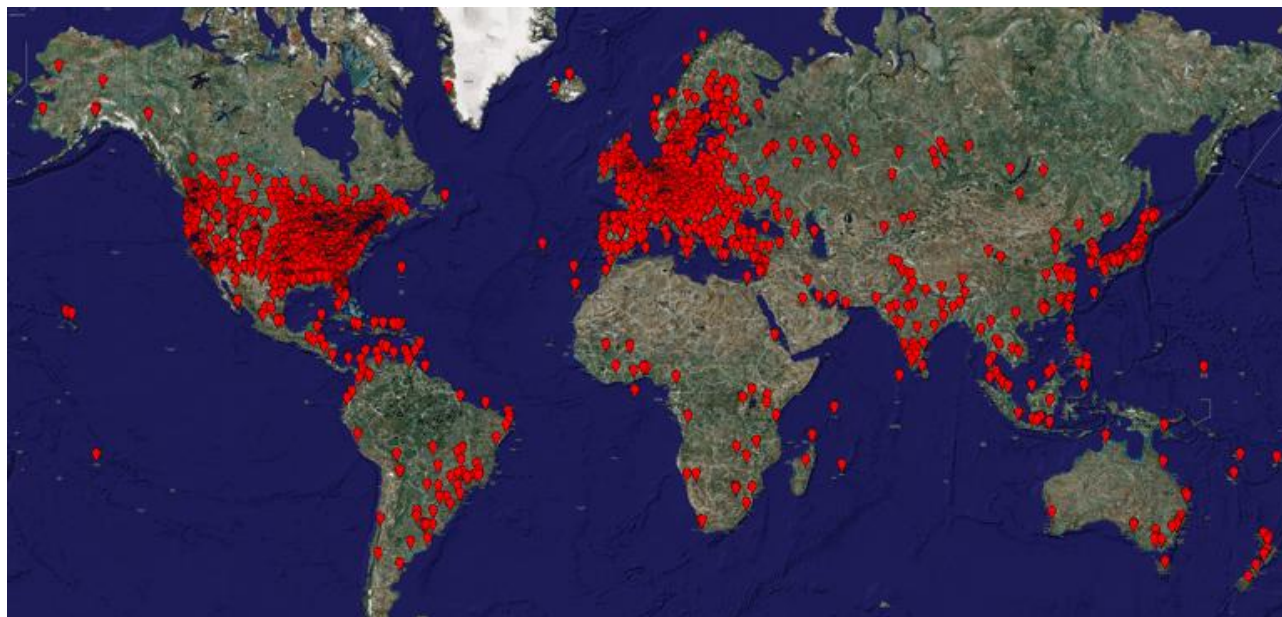
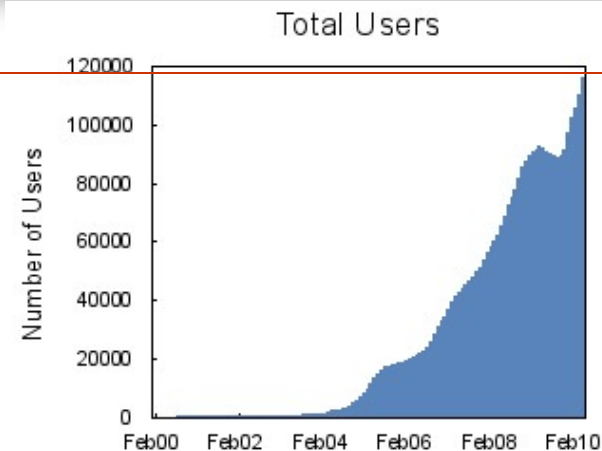
Users at all top 50 US Engineering Schools

19% of all .edu domains

116 classes at 76 institutions in 2009

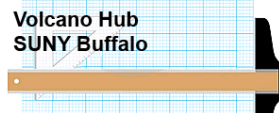
333 International Educational Institutions

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

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

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

- 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

- 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

- 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