Web-Based Simulations and Remote Access Visualization Tools for Science and Engineering Programs

July 27, 2022 (2:15 – 3:00 pm)

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Web-Based Simulations and Remote Access Visualization Tools for Science and Engineering Programs

Teaching and learning new and emerging technologies require state-of-the-art laboratories with expensive equipment. However, such facilities require large financial resources and time restraint to implement. Use of web-based simulation and remote access visualization tools enhance students' learning and teaching of new and complex concepts without using expensive equipment. The proposed workshop will discuss application of web-based simulation tools and remote-access visualization (RAIN, Nanohub, Physicell, Phet, Compucell3D, PV Systems tools) for teaching, research, and collaboration in areas such as nanotechnology, material science, environmental science, electrical engineering, biological sciences, physics, chemistry, and photonics.

Ahmed Khan, Professor/Fulbright Scholar, Fulbright / World Learning Inc, World Learning Inc, Washington, DC, Oak Brook, IL; **Sala Qazi**, Professor Emeritus, SUNY Polytechnic Institute, Utica, NY, Hollywood, MD; **Atilla Ozgur Cakmak**, Assistant Professor, Grand Valley State University, Grand Rapids, MI

Order of Presentation

- Fusion of 4the Industrial Revolution (4IR)Technologies: Challenges and Opportunities for Academia
- Online Tools for Visualization and Simulations
  - NanoHub
    - Examples of simulations using nanoHub
  - Phet Interactive Simulations
  - Physicell
  - CompuCell3D
    - Examples of Simulation of Covid-19 Virus
  - RAIN: Remote Accessible Instruments for Nanotechnology
    - AFM Application for visualization of Viruses
  - PV Systems modeling and simulation tools
- Best Practices and Sample Experiments to Support Lectures at PSU & GVSU
    - Examples of XPS & XRD
- Student Reception and Applicability
- First Time use tips for Instructors
- Conclusion
- Q & A

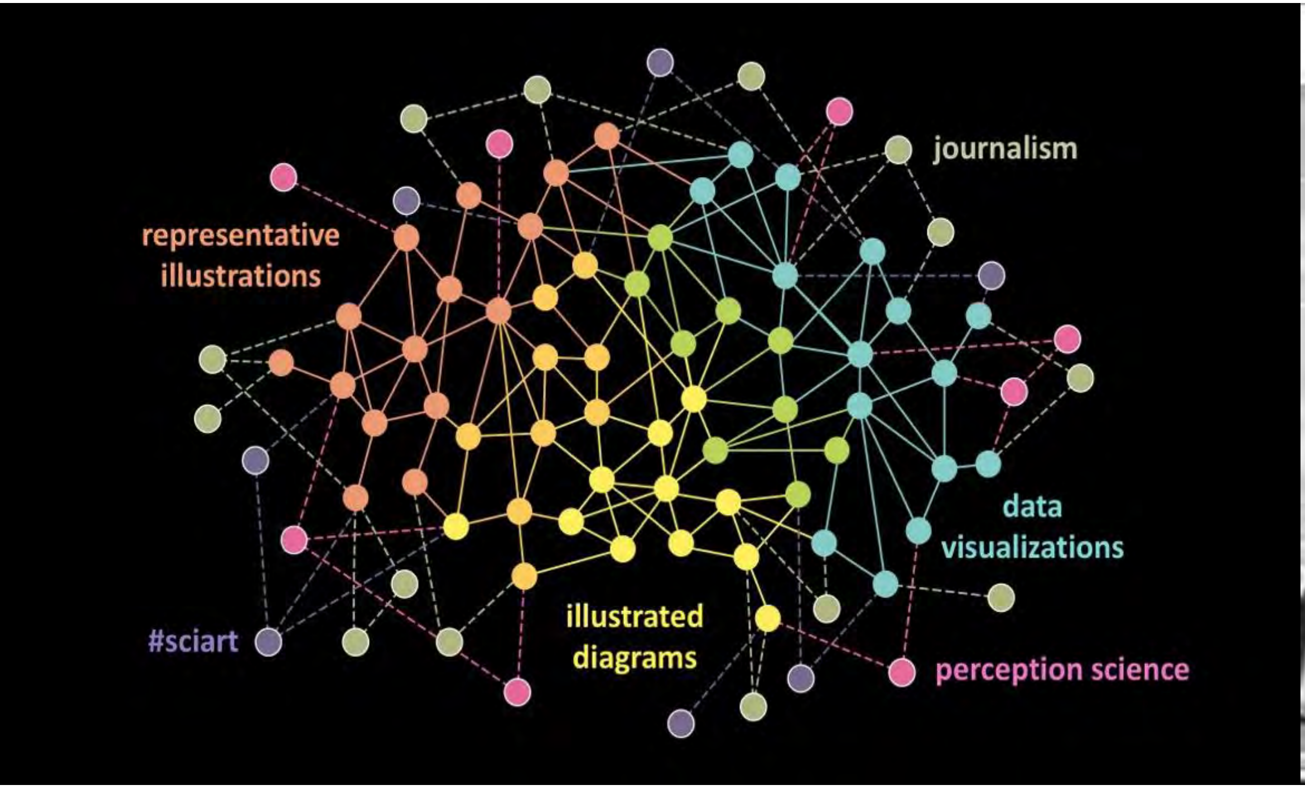
This workshop will discuss application of online simulation tools and remote access visualization for teaching, research and collaboration in the areas of

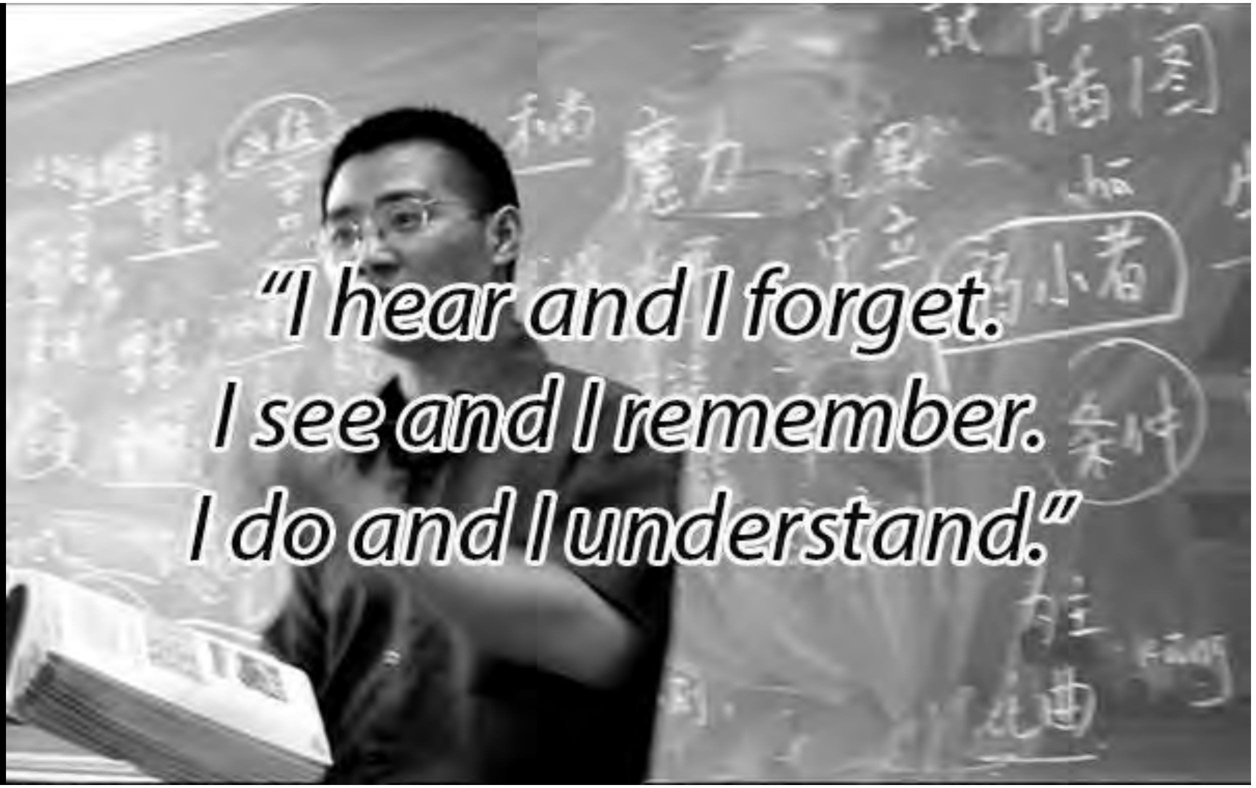
Nanotechnology, Physics, Math, Earth Sciences, and Biological Sciences

- Remote Accessible Instruments for Nanotechnology (RAIN): https://www.nano4me.org/remoteaccess
- NoanoHUB: https://nanohub.org/
- Phet Interactive Simulations: https://phet.colorado.edu/
- Physicell: http://physicell.org/
- 3DCompucell: https://compucell3d.org/

- **Best Practices and Sample Experiments to Support Lectures at PSU/GVSU**

Visualization and Simulation Enhances Student Learning





https://blogs.scientificamerican.com/sa-visual/visualizing-science-illustration-and-beyond/

4IR…Changing World…Education…Intellectual Capital

Empires of the Future...

"The empires of the future will be the empires of the mind."

--- *Sir Winston Churchill*

4IR…Changing World…Education…Intellectual Capital

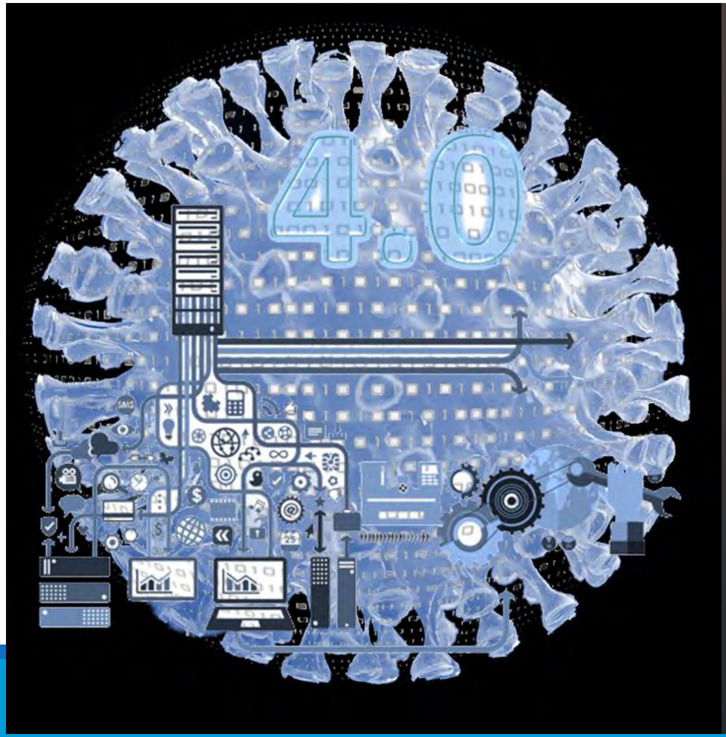
- **The emerging technologies of the 4th Industrial Revolution (4IR) are quietly and dramatically changing society; the way we interact with others, live, work, and educate our students at local, national, and international levels.**
- **Such changes are enabled by emerging technologies like Artificial Intelligence (AI), big data, Internet of Things (IoT), Augmented Reality, Blockchain, Robotics, Drones, Nanotechnologies, Genomics & Gene Editing, Quantum Computing, and Smart Manufacturing.**

- **The fusion of these technologies is impacting all sectors across the globe at an unprecedented speed.**

  - ***How will all stakeholders deal with 4IR's short-term and long-term benefits, limitations, uncertainties, and risks?***
  - ***How do we prepare our students and educators for the 4IR world?***
  - ***What resources will be need?***


High Impact Technology Exchange Conference
HI TEC
July 25–28, 2022
Grand America Hotel
Salt Lake City, UT


4th
Industrial
Revolution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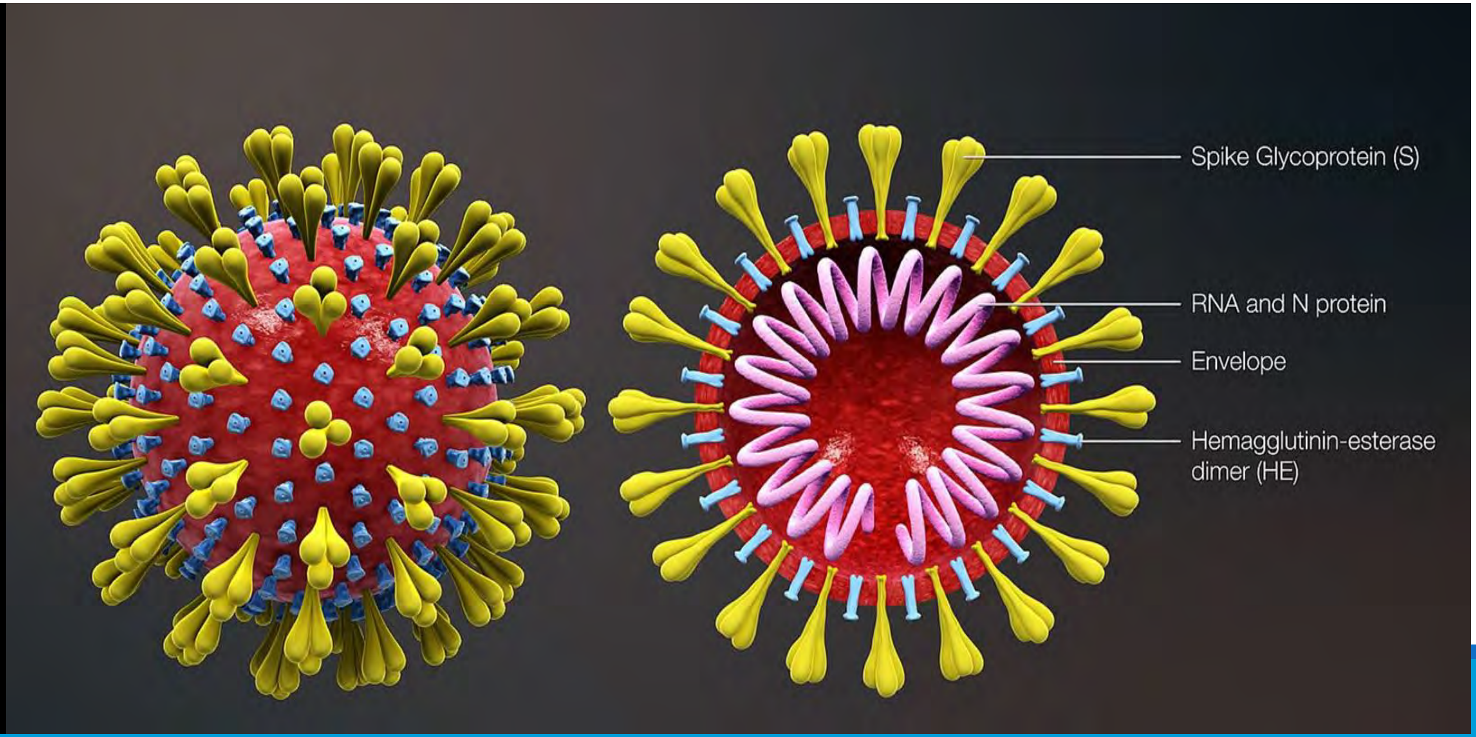
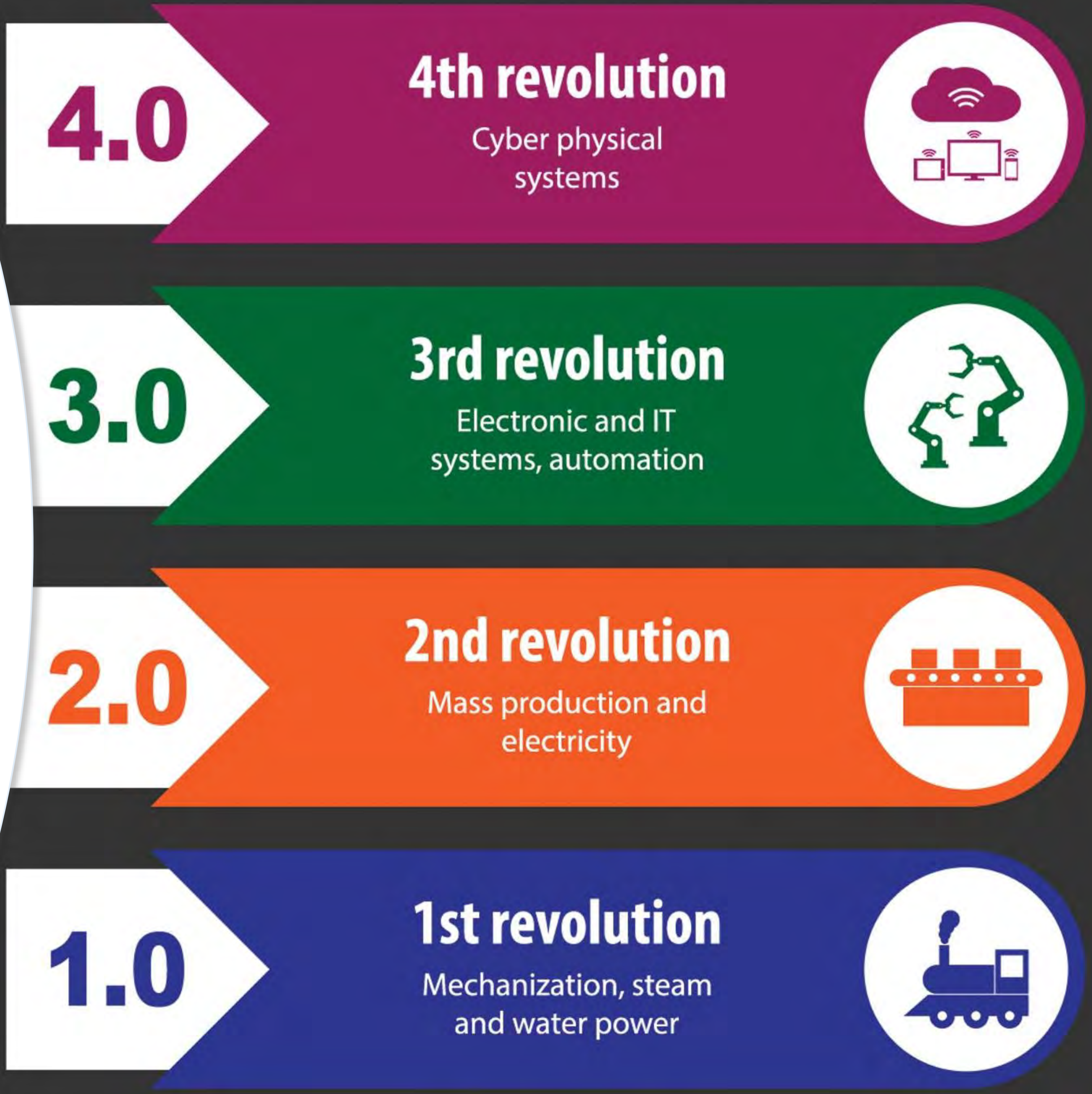

Spike Glycoprotein (S)
RNA and N protein
Envelope
Hemagglutinin-esterase
dimer (HE)

The Industrial Revolutions

Fourth Industrial Revolution is, *however, fundamentally different. It is characterized by a range of new technologies that are fusing the physical, digital and biological worlds, impacting all disciplines, economies and industries, and even challenging ideas about what it means to be human.*

Different Continents & Countries

Different IR Numbers 1.0 2.0 3.0 4.0



"The Fourth Industrial Revolution has the potential to empower individuals and communities, as it creates new opportunities for economic, social, and personal development. But it also could lead to the marginalization of some groups, exacerbate inequality, create new security risks, and undermine human relationships."

--- Klaus Schwab

4IR
Pros & Cons

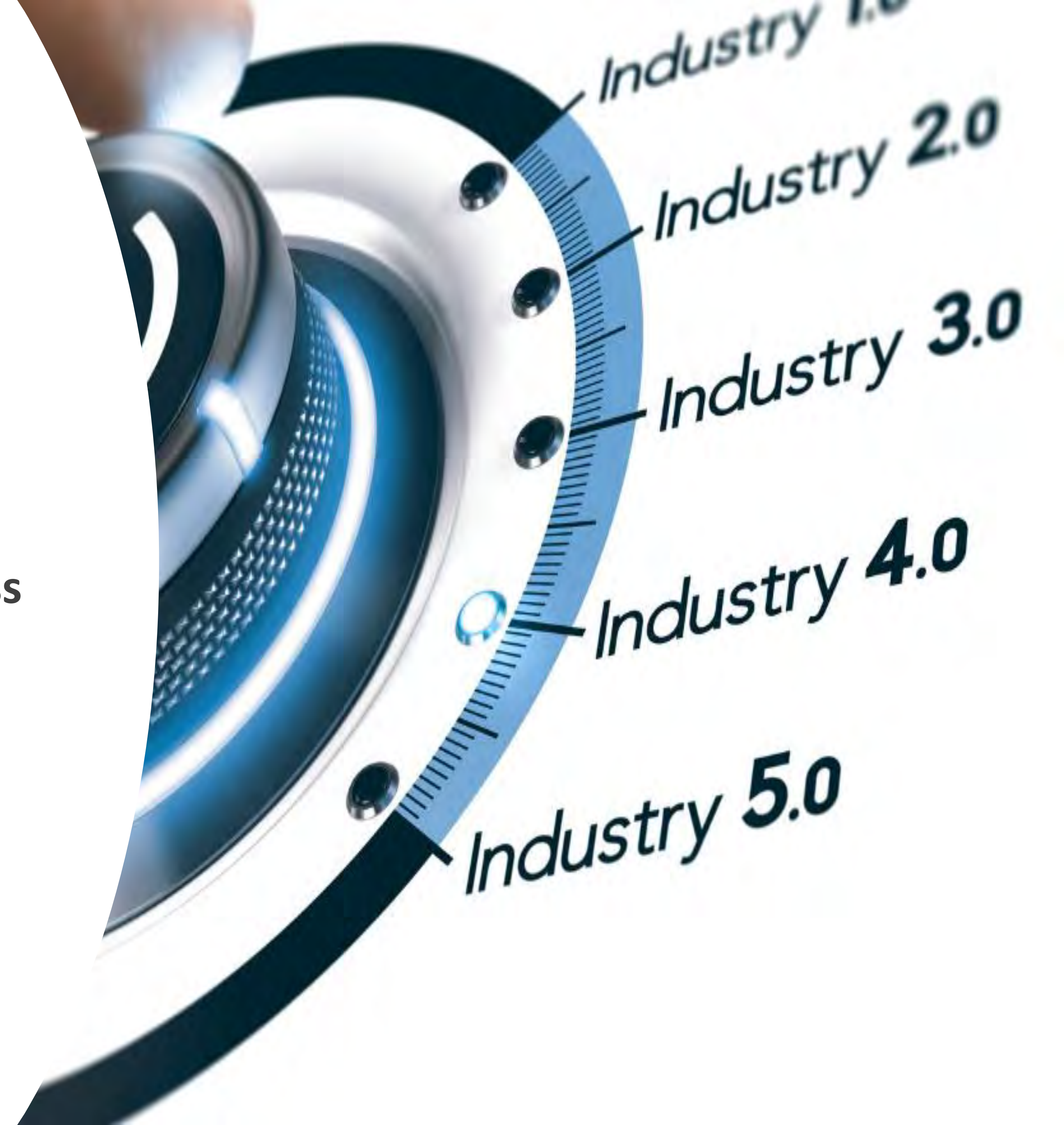
Pro

1. Higher Productivity
2. Improved Quality of Life
3. New Markets
4. Lower barrier to creating new business opportunities

Cons

1. Inequality
2. Cyber security risks
3. Core industries disruptions
4. Ethical Issues

Source: https://www.lightsondata.com/pros-cons-4th-industrial-revolution/



Fusion of 4IR Technologies: Challenges and Opportunities for Academia

- The exponential rate of technological advances and the convergence of scientific knowledge are shrinking the time to remake the world.

- Today, a knowledge- and innovation-based economy is essential for the development of nations around the globe.

- For nations to maintain a technological edge, the technical competency of graduates has become paramount.

- This transition towards the new economic realities has also created a paradigm shift in the modes of teaching and learning.

- The education system has been transformed into a “lifelong learning” model. In this model, the traditional role of a professor has also changed—from the primary mode of providing information to creating an interactive dialogue to foster teaching/learning.

Fusion of 4IR Technologies: Challenges and Opportunities for Academia

The convergence of multiple disciplines & diffusion of Technologies has put new demands on educators, students and academic institutions.

As the pace of technological change becomes faster, a new paradigm is required in the domains of teaching and learning.

The following factors are becoming transformative:

- 21st century graduate skills sets
- Emergence of global standards for product development
- Developments in the science of learning/teaching (pedagogy)
- Awareness of social and ethical implications of technology (STS)
- E-learning and modes of delivery
- Faculty technical and professional currency

Fusion of 4IR Technologies: Challenges and Opportunities for Academia

Emerging 4IR Technologies and New Demands on Skill-sets of Graduates

- The global marketplace seeks up-to-date technical knowledge and skills.
- The pace of technological change also imposes new challenges for faculty development and technical currency of academic programs.
- To be successful in the 21st century workplace, graduates must acquire digital-age technical literacy.
- Graduates are not only expected to understand the theory behind state-of-the-art technologies, but also exhibit *hands-on and analytical problem solving*, *expert thinking*, *awareness of social and ethical implications of technology*, *interpersonal skills*, *teamwork*, *and* *cross-disciplinary communication skills.*

Top 10 Emerging Technologies

1. Fuel cell vehicles
2. Next-generation robotics
3. Recyclable thermoset plastics
4. Precise genetic engineering techniques
5. Additive manufacturing
6. Emergent artificial intelligence
7. Distributed manufacturing
8. ‘Sense and avoid’ (AI) drones
9. Neuromorphic technology
10. Digital genome

https://www.weforum.org/agenda/2015/03/top-10-emerging-technologies-of-2015-2/

MIT Technology Review (2021)

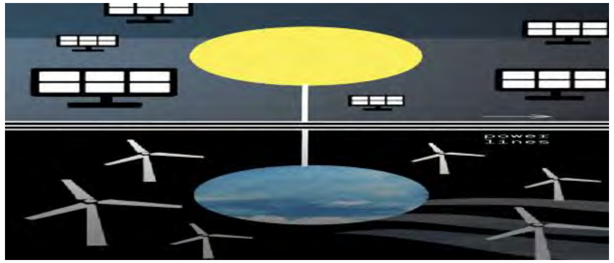
Top 10 Emerging Technologies

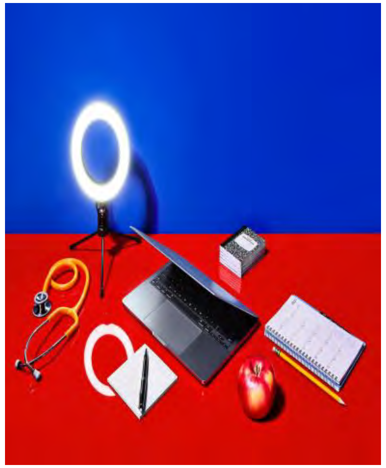
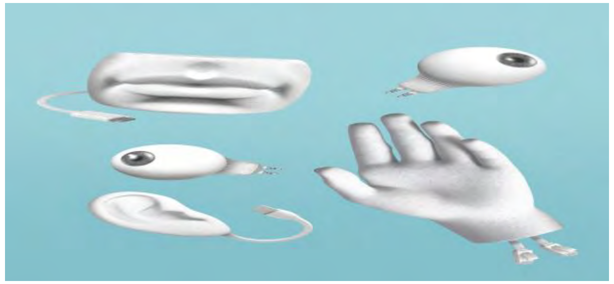
- Messenger RNA vaccines
- GPT-3 Natural language computer models (AI)
- Data trusts to ensure user privacy
- Green hydrogen replacement for fossil fuel
- Lithium-metal batteries to increase the range of EVs
- Digital contact tracing to curb the spread of Covid-19 pandemic
- Hyper-accurate positioning to improve the positioning accuracy to 1-2 m
- Multi-skilled AI to improve its senses
- TikTok's "For You" algorithms to promote a niche identity or interest
- Remote everything using online technologies



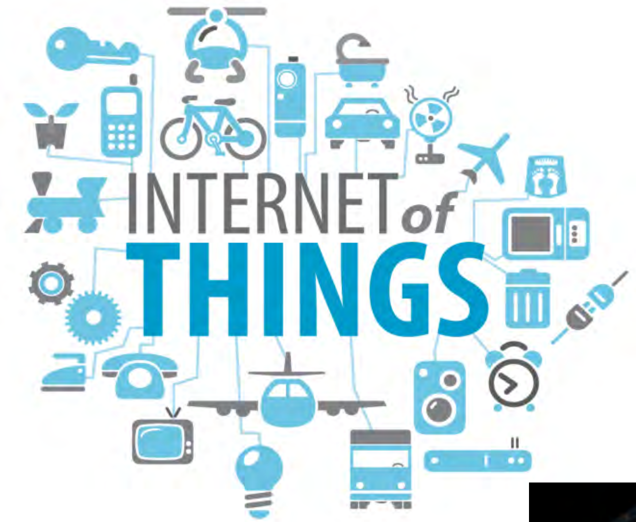


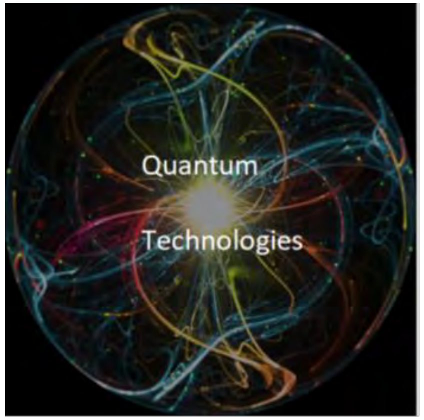


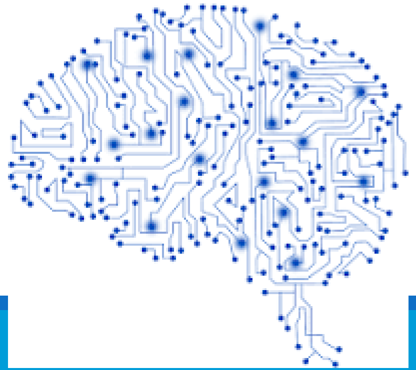


Emerging Technologies







Modern AI Theory of Evolution

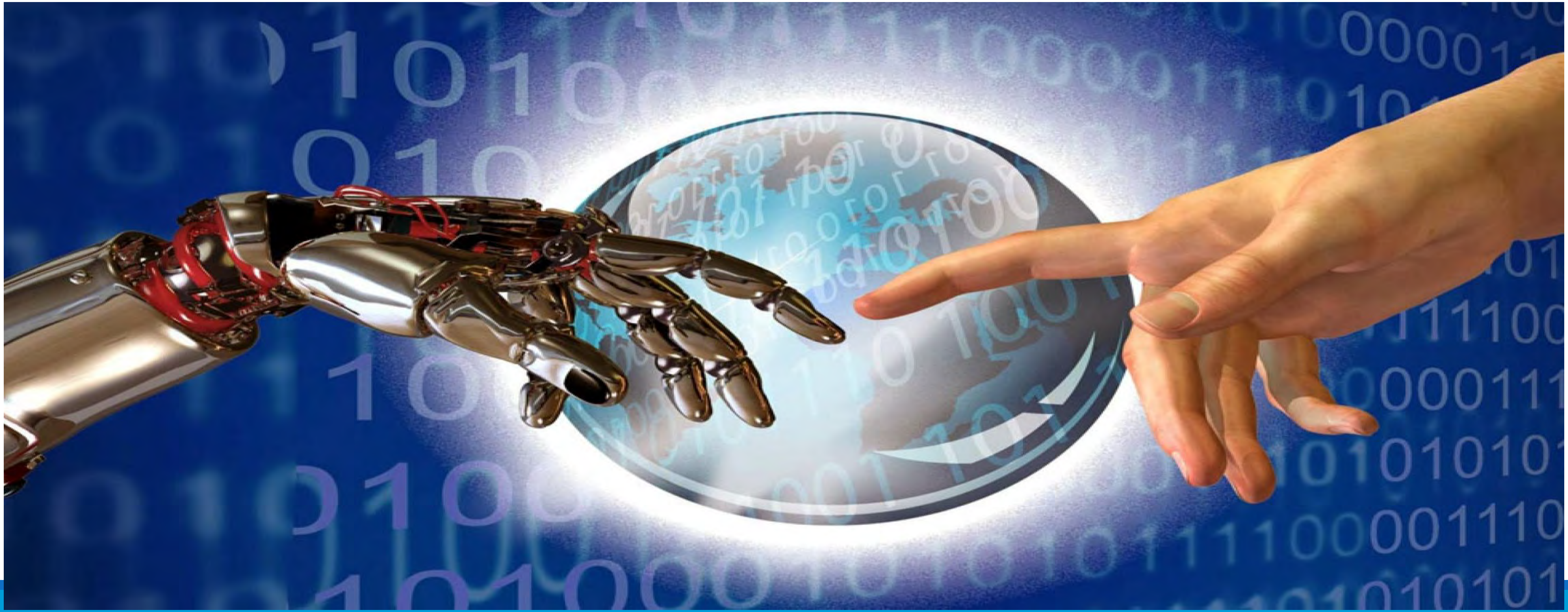
Computer	Basic Robot	Programmable Robot	Human-Like	Super Human-Like
Number Cruncher	Special Purpose	Foundational AI	Augmented AI	Strong AI
Computation	Repeated Tasks	Machine Learning	Deep Learning	Conscience?
1950's	1990's	2010's	2030's	2040's+

Wisdom

Love

Soul

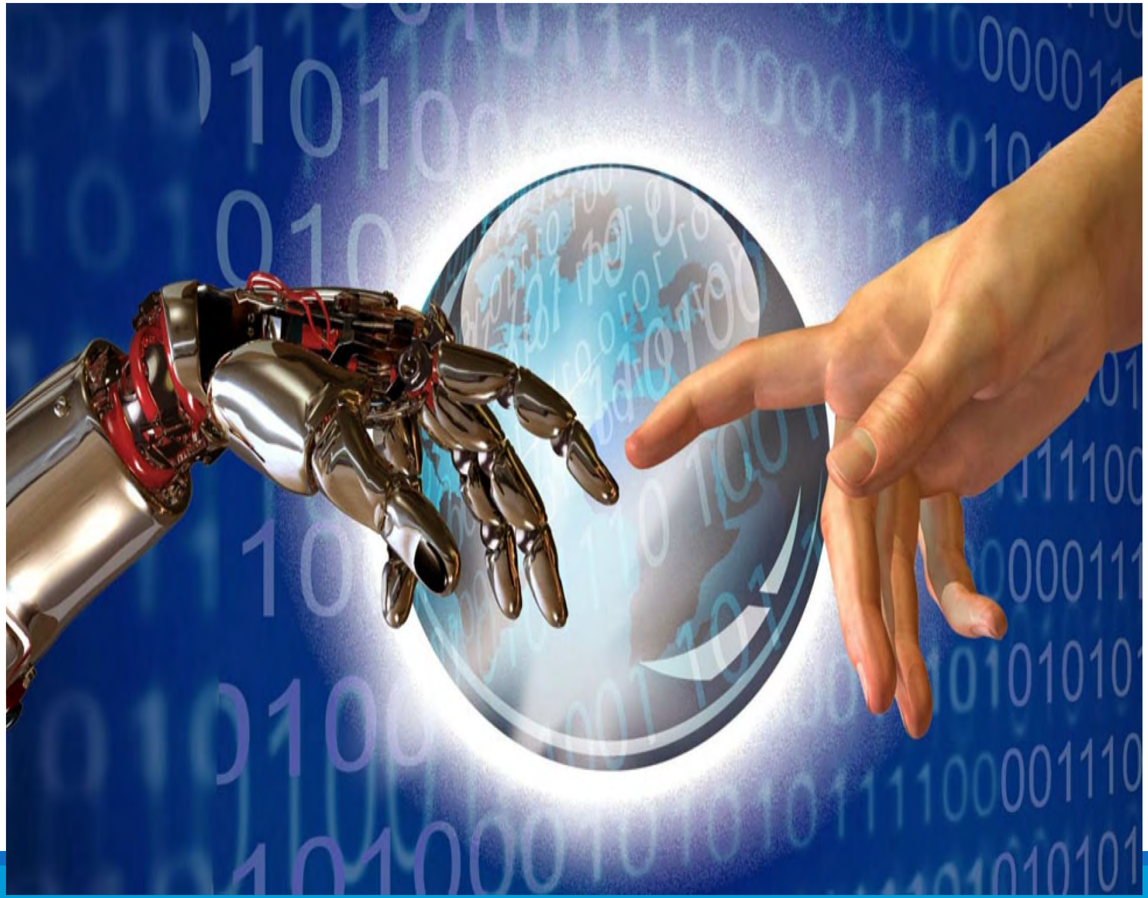
Man-Machine Interactions



Problems & Issues

Man-Machine Interactions

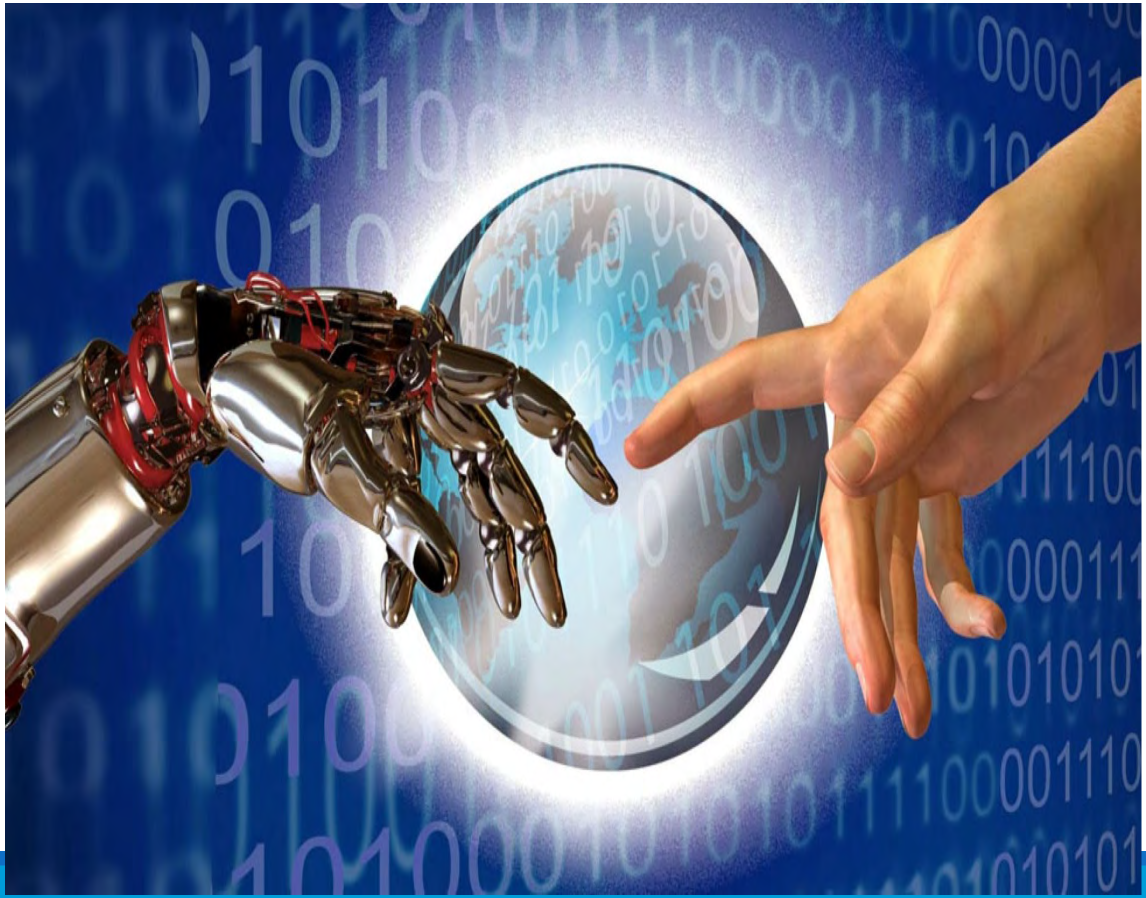
- Data Security & Digital Rights
- Manipulation of Digital Data (Fake News)
- Social Media Activism
- Accountability & Transparency
- Ethical Implications



Intended and Unintended Consequences of 4IR Technologies

- All new and emerging technologies have dual nature: positive and negative impacts or intended and unintended consequences.

- One of the biggest challenge of the 4IR is:
- How can we maximize the intended benefits of technology while limiting the unintended consequences of technology?



Emerging 4IR Technologies

Nanotechnology, Robotics and Artificial Intelligence (AI)

Web Based Simulations and Remote Access Visualization Tools for Science & Engineering Programs

Key Challenge

- Teaching, Learning and Research in new and emerging technologies require state of the art laboratories equipped with expensive equipment and associated support facilities.

- However, such facilities also require large financial resources and time restraints to implement the requirements.

- Use of Web-based Simulation and Remote Access Visualization Tools enhance students' learning and teaching of new and complex concepts without physically using required expensive equipment.

Web Based Simulations and Remote Access Visualization Tools for Science & Engineering Programs

- Simulation method offers another major advantage. Itis task- and learner-neutral, it just models an object/system construction and operation or learning situation.

- Within simulation functionality, there are no curbs on the student's actions.

- Realistic simulations visualize processes occurring in the devices and enable students to observe the physical processes at different levels (from macroscopic to subatomic), analyze constraints between physical parameters, compare actual and virtual data, and much more.

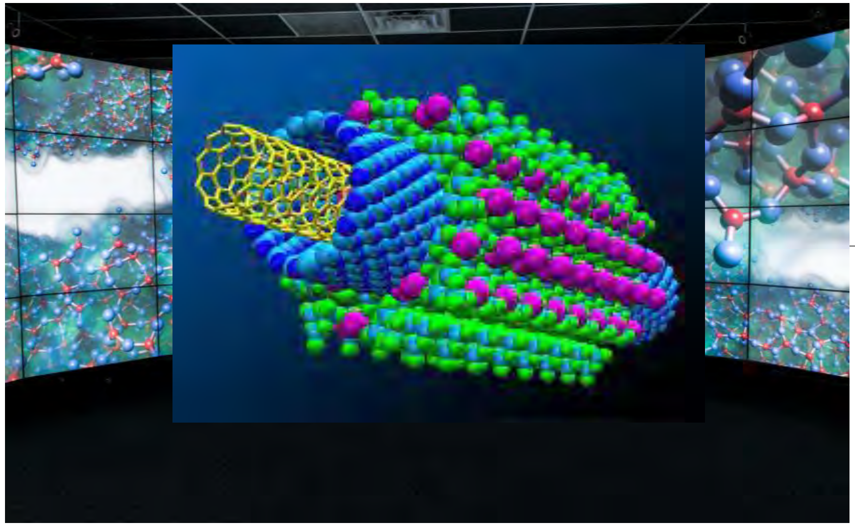
Web Based Simulations and Remote Access Visualization Tools for Science & Engineering Programs

Online simulation tools and remote access visualization provide viable platforms for teaching, research, and collaboration in the areas of nanotechnology, material science, environmental science, electrical engineering, biological sciences, physics, chemistry, photonics and much other areas.

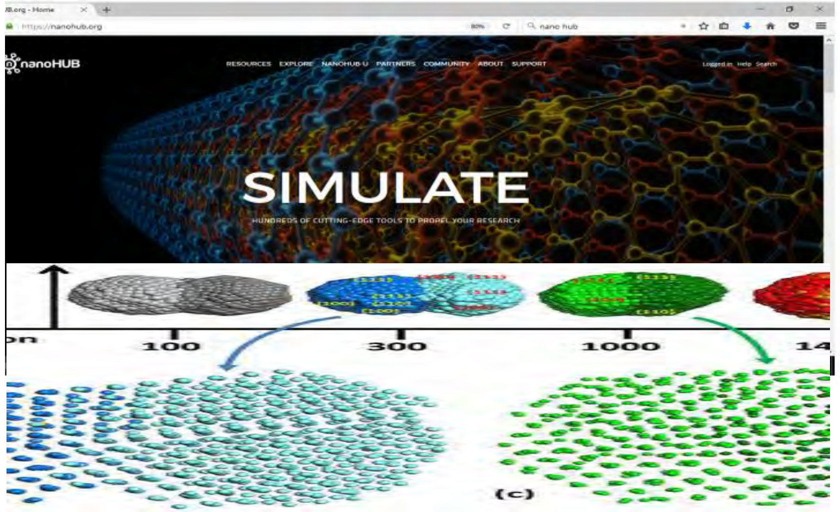
These tools include:

- **RAIN (Remote Access Instruments in Nanotechnology) 26 nodes for accessing visualization instruments**
- **NanoHub has 500+ simulation tools to simulate nanotechnology processes**
- **Phet Interactive offers Simulations for teaching Physical Sciences and Math**
- **CompuCell3D & Physicell offer flexible modeling platforms that allow simulations for biology, tissue engineering, and viruses including COVID19.**

Simulation



Crystal Viewer Tool
Nanohub.org



Simulation offers many advantages:

(a) allowing the user to modify system parameters and observe the outcomes without any harmful side effects

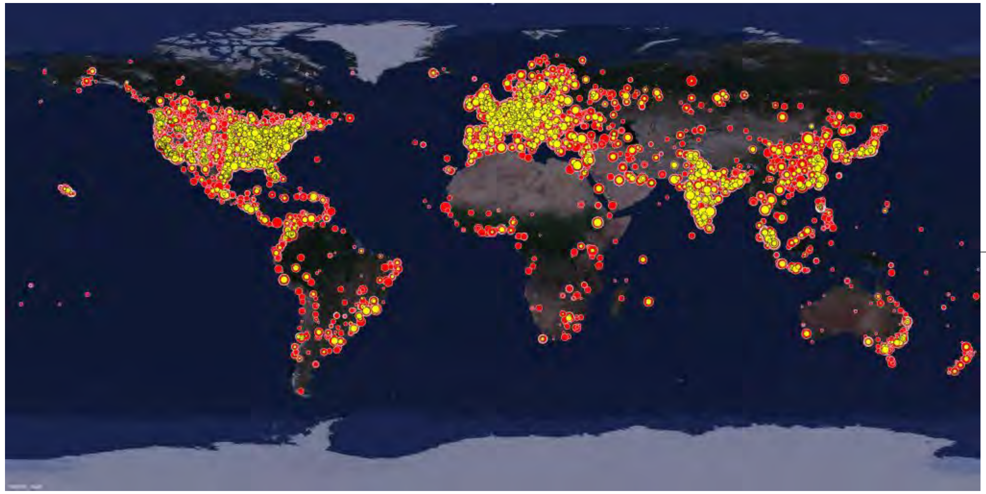
(b) eliminating component or equipment faults that affect outcomes

(c) supporting users progress at their own pace in discovery and understanding of concepts and issues,

and (d) enhancing the presentation of “dry” concepts by integrating theory and practice

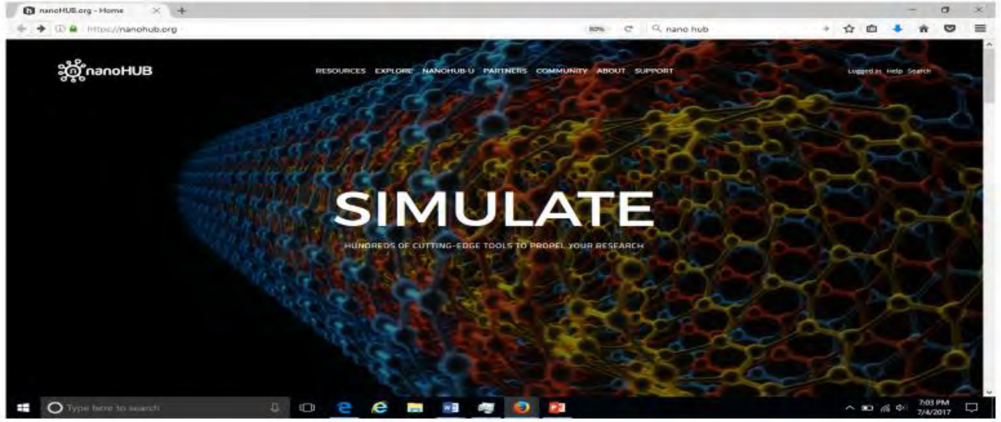
Learning through Visualization and Simulation at the Nanoscale

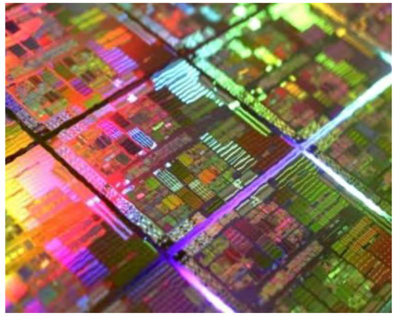
Nanohub.org

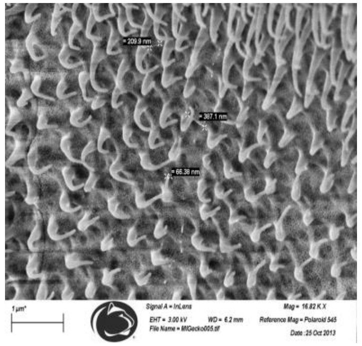


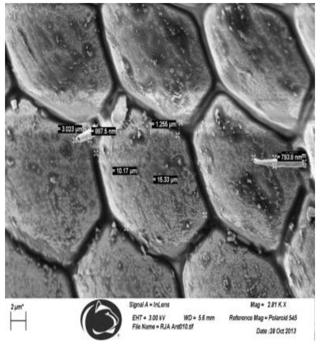
- Computing Cloud located at Purdue University
- 500+ simulation tools & apps
- 1.4 million users Worldwide
- 6500 resources

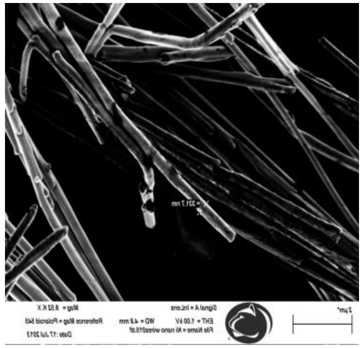
Crystal Viewer Tool
Nanohub.org



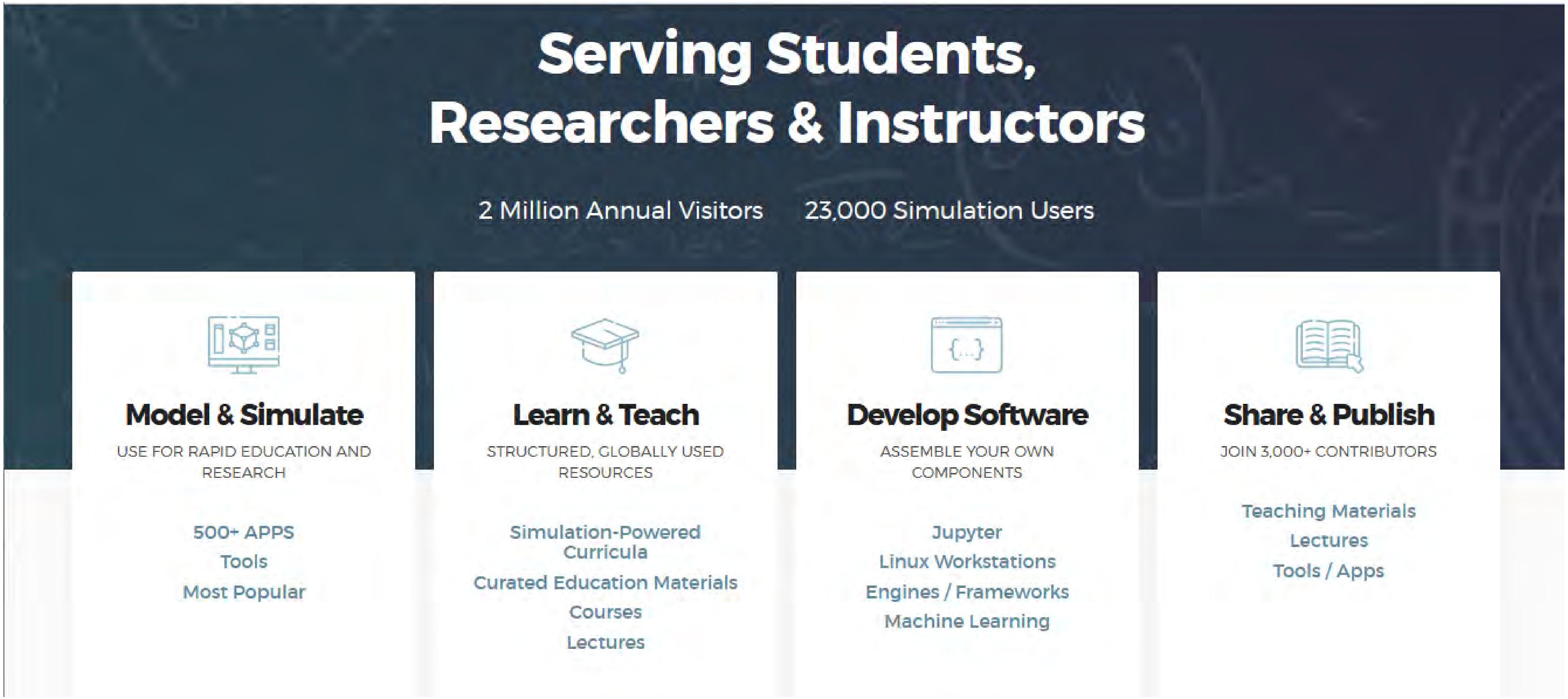








NanoHub


Serving Students,
Researchers & Instructors
2 Million Annual Visitors
23,000 Simulation Users
Model & Simulate
USE FOR RAPID EDUCATION AND RESEARCH
500+ APPS
Tools
Most Popular
Learn & Teach
STRUCTURED, GLOBALLY USED RESOURCES
Simulation-Powered Curricula
Curated Education Materials
Courses
Lectures
Develop Software
ASSEMBLE YOUR OWN COMPONENTS
Jupyter
Linux Workstations
Engines / Frameworks
Machine Learning
Share & Publish
JOIN 3,000+ CONTRIBUTORS
Teaching Materials
Lectures
Tools / Apps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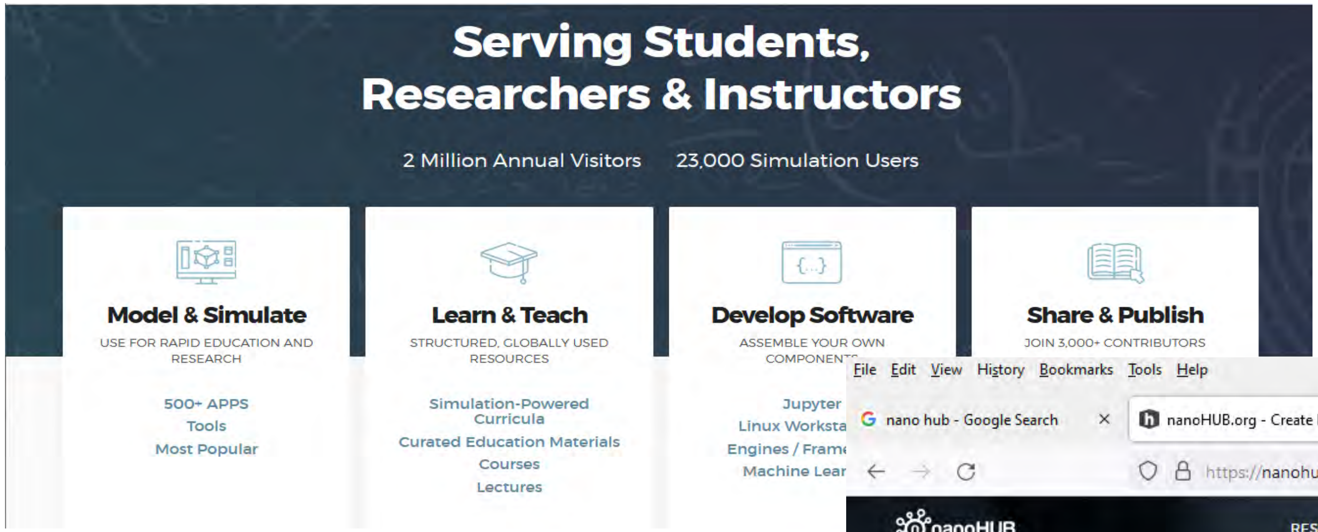
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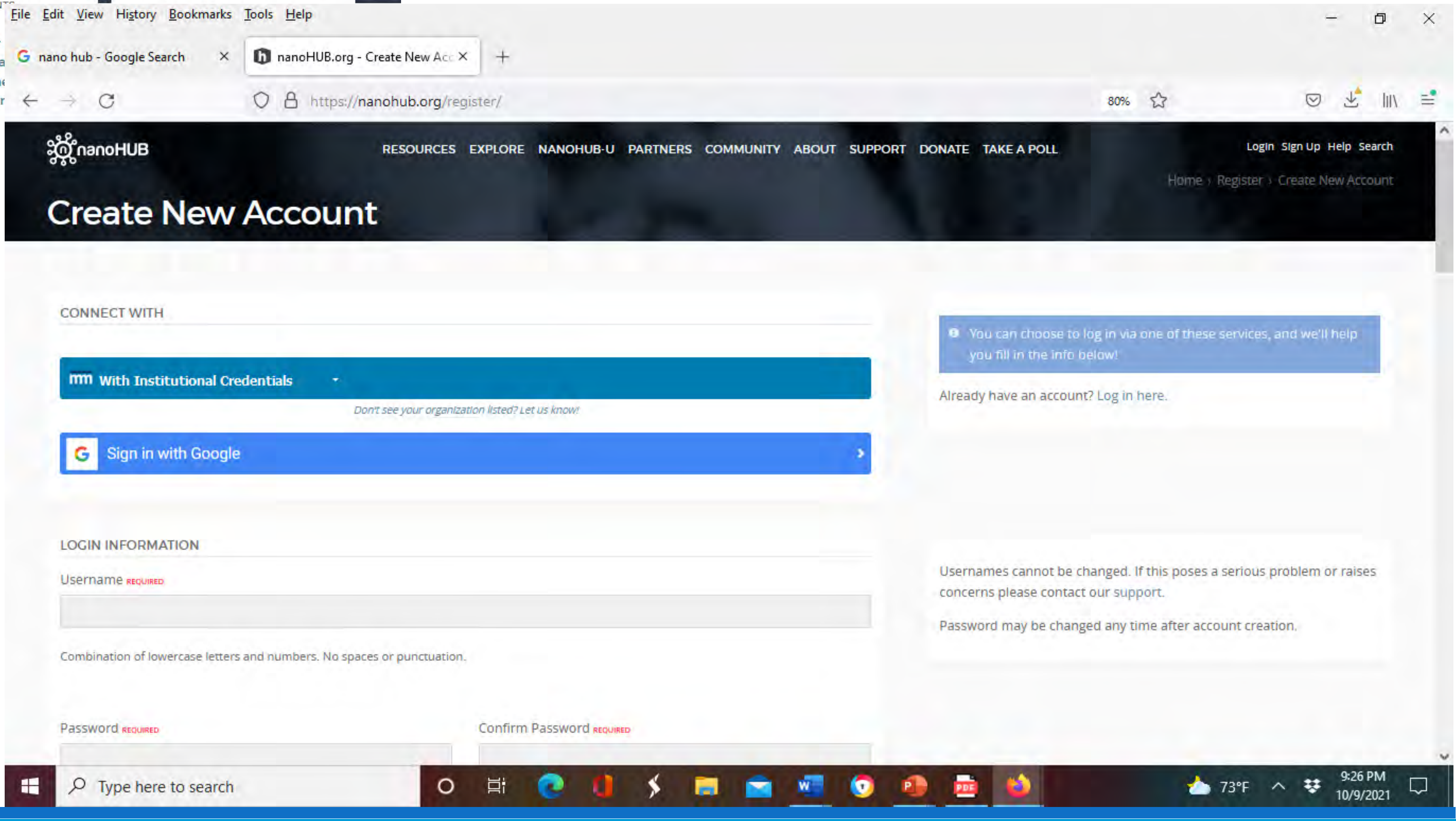

File Edit View History Bookmarks Tools Help
nano hub - Google Search
https://nanohub.org/register/
nanoHUB
RESOURCES EXPLORE NANOHUB-U PARTNERS COMMUNITY ABOUT SUPPORT DONATE TAKE A POLL
Login Sign Up Help Search
Home › Register › Create New Account
Create New Account
CONNECT WITH
With Institutional Credentials
Don't see your organization listed? Let us know!
Sign in with Google
You can choose to log in via one of these services, and we'll help you fill in the info below!
Already have an account? Log in here.
LOGIN INFORMATION
Username REQUIRED
Combination of lowercase letters and numbers. No spaces or punctuation.
Usernames cannot be changed. If this poses a serious problem or raises concerns please contact our support.
Password may be changed any time after account creation.
Password REQUIRED
Confirm Password REQUIRED
Type here to search
73°F
9:26 PM
10/9/2021

NanoHub

NanoHub: Top Tools by Simulation Users

nanoHUB

RESOURCES EXPLORE NANOHUB-U PARTNERS COMMUNITY ABOUT SUPPORT DONATE TAKE A POLL

Logged in Help Search

Home › Usage › Tools

Usage: Tools

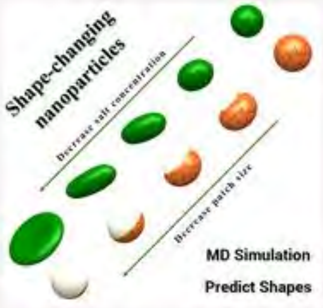
Overview Tools

Show data for: Top Tools by Simulation Users | Jul 2020 - Jun 2021 | View

Top Tools by Simulation Users

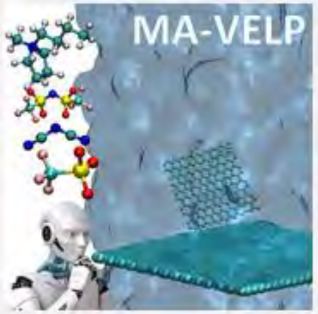
#	Tool	Simulation Users	Percent
1	PN Junction Lab	2,293	10.17%
2	ABACUS - Assembly of Basic Applications for Coordinated Understanding of Semiconductors	1,966	8.72%
3	PN Junction Lab (New Interactive Front End)	1,534	6.80%
4	Crystal Viewer Tool	1,504	6.67%
5	Crystal Viewer Lab (New Interactive Front End)	1,281	5.68%
6	MOSFet	1,092	4.84%
7	a TCAD Lab	1,072	4.75%
8	Machine Learning for Materials Science: Part 1	1,034	4.58%
9	DFT calculations with Quantum ESPRESSO	1,000	4.43%

NanoHub: Featured Resources



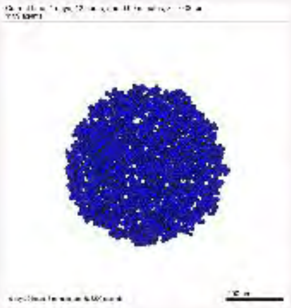
Nanoparticle Shape Lab

nanoBIO tool reveals novel ways of controlling design of shape-changing nanoparticles. The findings could be used in the design of smart drug-delivery containers and have applications in nanomedicine and the development of new reconfigurable materials.



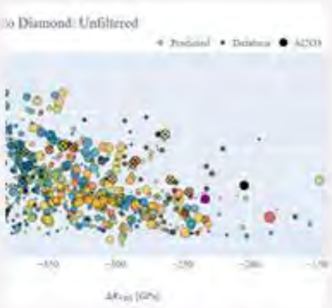
2D Materials Liquid Exfoliation

Machine learning tool for screening and analysis of solvent performance in liquid phase exfoliation of 2D materials using simulation data.



Winter Interactive nanoBIO Workshop

The Winter Interactive nanoBIO Workshop will teach students and researchers to understand a variety of biological problems using nanoHUB's easy-to-use cloud-based simulation tools.



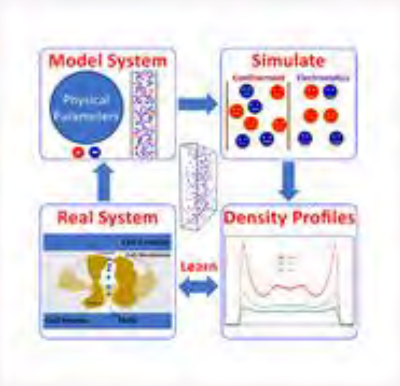
Machine Learning Modules

Explore and use educational modules for data science and machine learning in engineering. Each module consists of a recorded lecture, hands-on tutorial, and homework assignment with online simulations.

Gr-ResQ

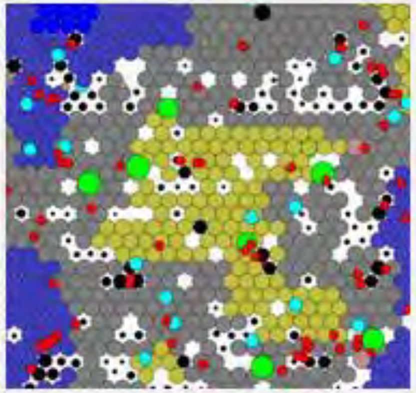
A comprehensive database of recipes and results of graphene synthesis by chemical vapour deposition, as well as a suite of software tools to analyze the database.

NanoHub: Featured Resources



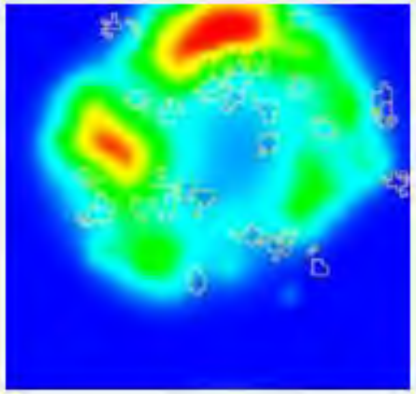
Ions in Nanoconfineme

This app empowers users to simulate ions confined between material surfaces that are nanometers apart, and extract the associated ionic structure. The app facilitates investigations for a wide array of ionic and environmental parameters



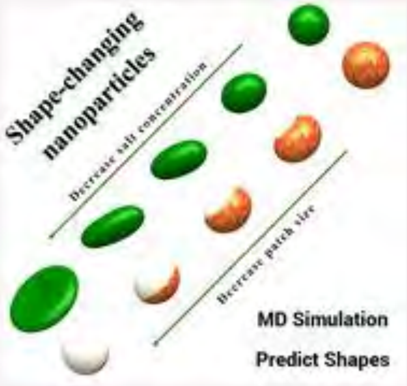
PhysiCell for COVID-19

This model simulates viral dynamics of SARS-CoV-2 (coronavirus / COVID19) in a layer of epithelium and an immune response. It is being rapidly prototyped and refined with community support.



COVID-19 Virtual Tissue Model

Built on the sophisticated CompuCell3D framework, the COVID-19 Virtual Tissue Model provides a predictive multiscale modeling framework that integrates



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NanoHub: Simulation Tools

SIMULATE

explore the powerful tools at your fingertips

Jupyter Notebook

Starts the Jupyter notebook server using the latest installed release of anaconda.

Workspace

Development workspace

a TCAD Lab

An Assembly of TCAD tools for circuit, device, and process simulation

nanoDDSCAT+

Combines the Discrete Dipole Scattering (DDSCAT) tool with the DDAConvert tool for a single workflow for custom shapes.

MIT Atomic-Scale Modeling Toolkit

Tools for Atomic-Scale Modeling

NanoHub: Simulation Tools

SIMULATE

explore the powerful tools at your fingertips

Purdue ME 581-Numerical Methods in Engineering Using Jupyter Notebooks

Jupyter notebooks with an introduction to python and examples for Numerical Methods in Engineering.

Crystal Viewer Tool

Visualize different crystal lattices and planes

ABACUS - Assembly of Basic Applications for Coordinated Understanding of Semiconductors

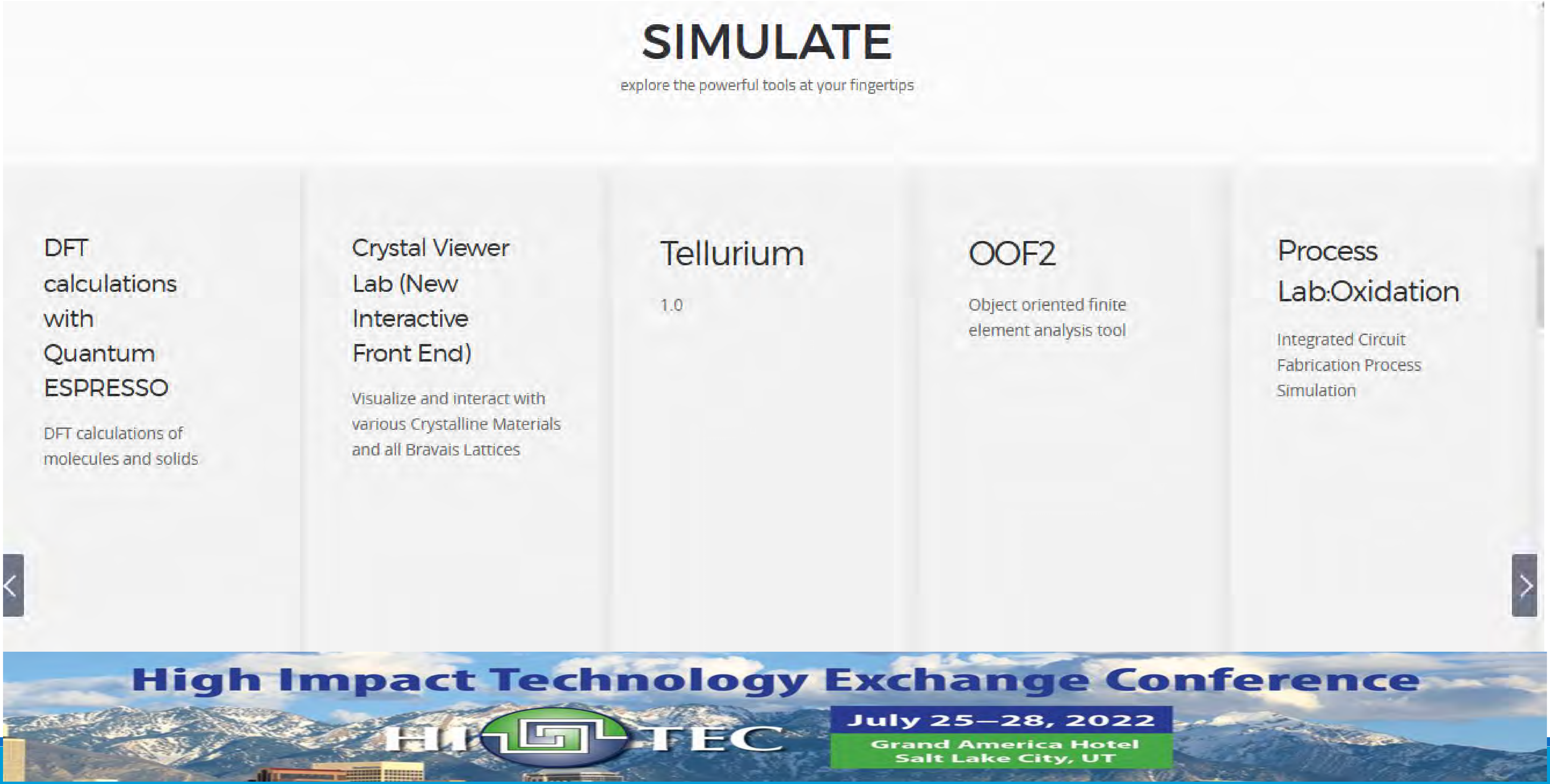
CompuCell3D v4 Main Tool

Base tool for CompuCell3D version 4 and greater. Allows running any of the demos included with CC3D (/CompuCell3D_Demos /Demos)

Polymer Modeler

Build thermoplastic polymer chains and run LAMMPS to relax the chains and study mechanical properties

NanoHub: Simulation Tools



NanoHub: Resources

EXPLORE

a range of resources at your disposal

SERIES
NCN Nanomaterials: Courses

COURSES
Illinois MATSE 280: Introduction to Engineering Materials

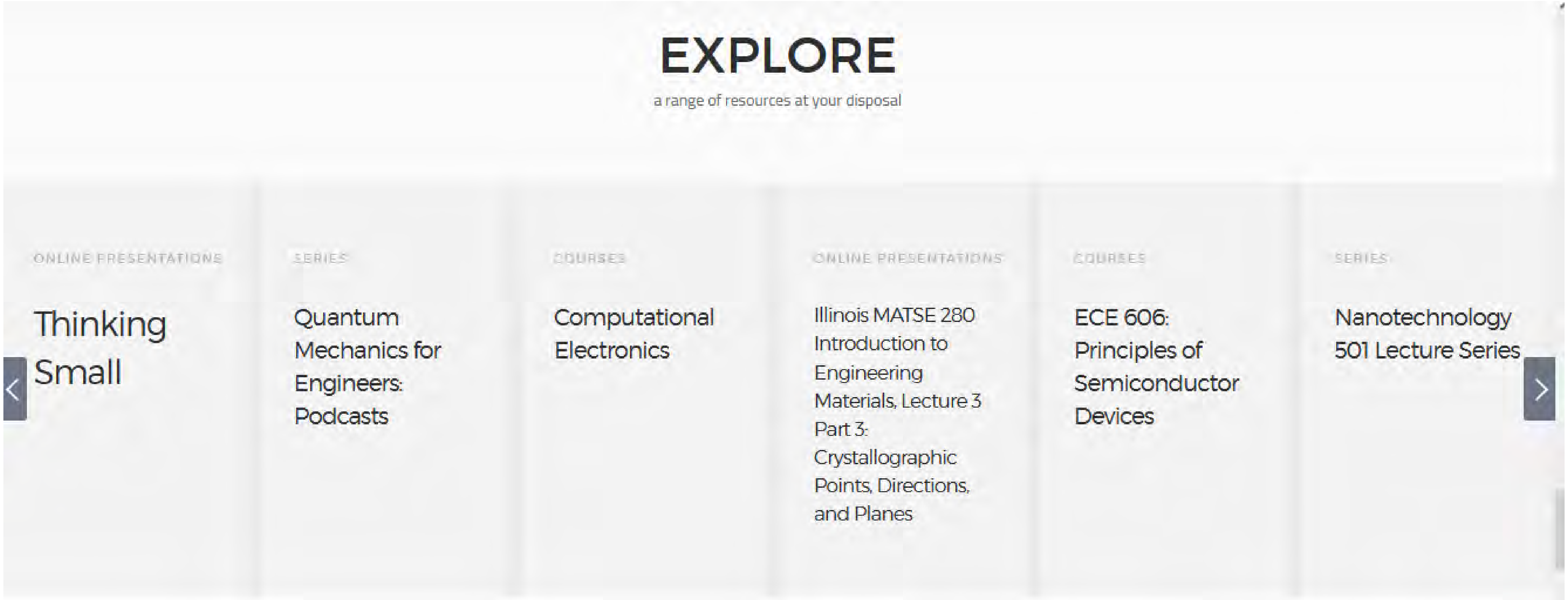
TEACHING MATERIALS
Renewable Energy Sources

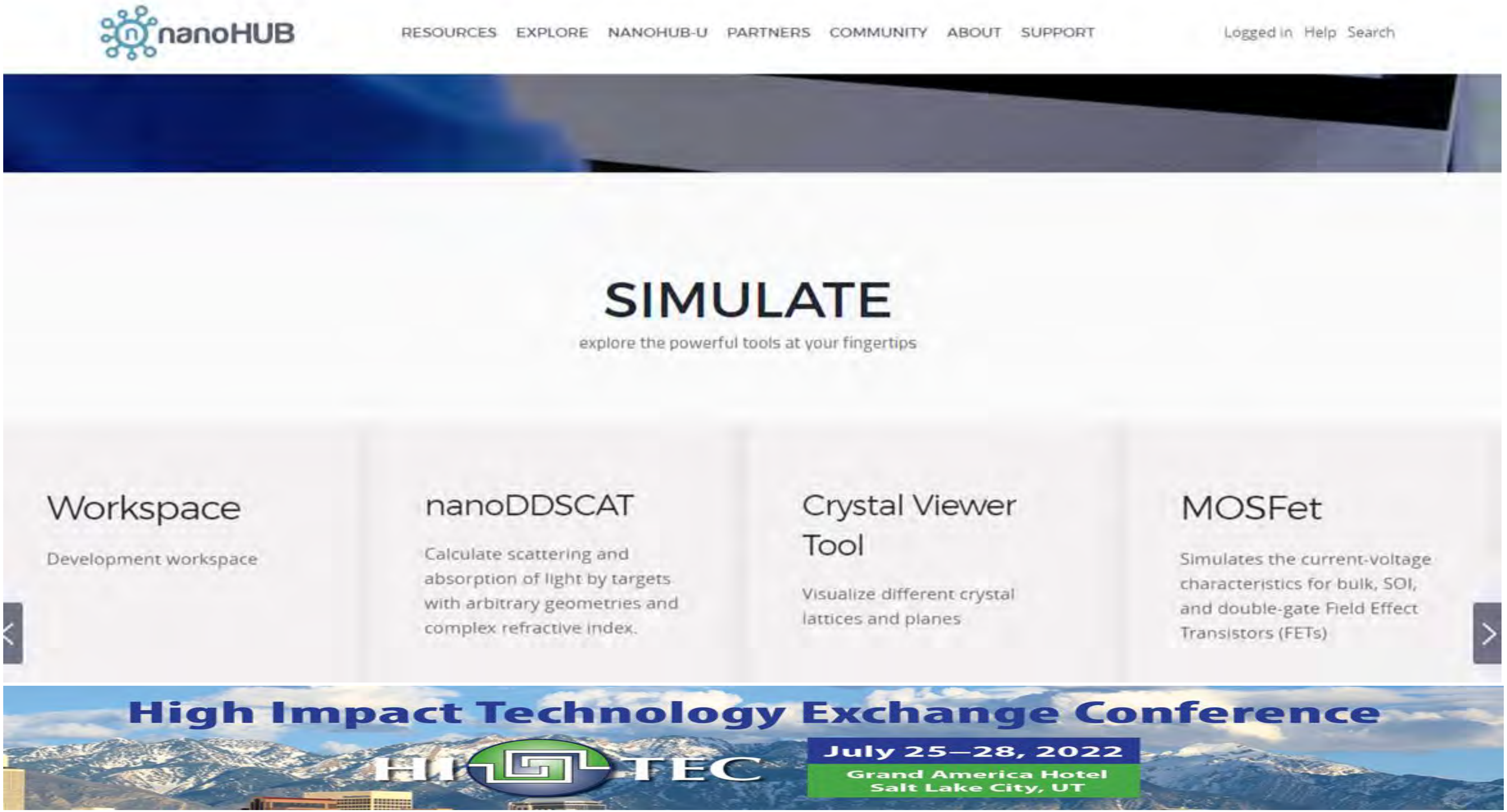
SERIES
Introductory Seminars on What is Nanotechnology?

SERIES
NCLT Seminar Series

SERIES
Electronics from the Bottom Up (roll-up)

NanoHub: Resources

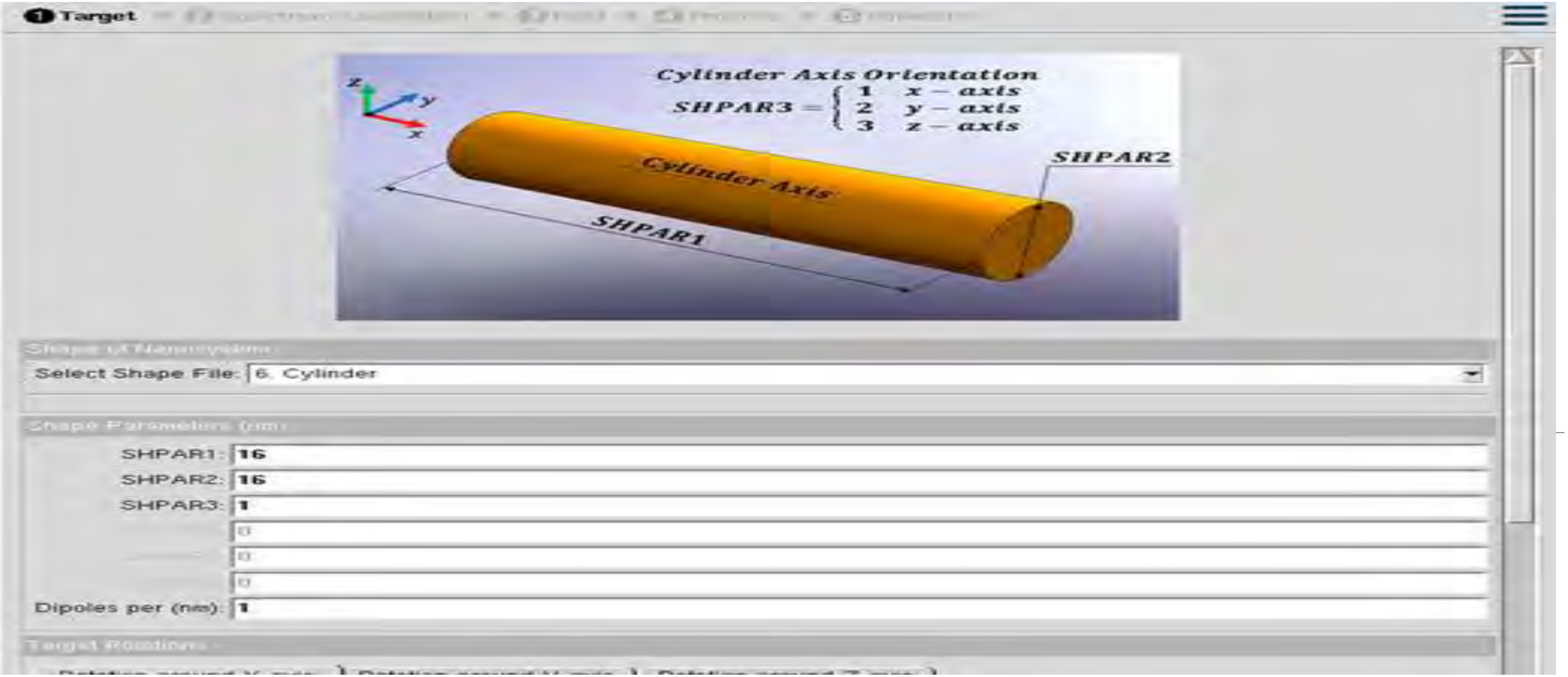



nanoHUB
RESOURCES EXPLORE NANOHUB-U PARTNERS COMMUNITY ABOUT SUPPORT
Logged in Help Search
SIMULATE
explore the powerful tools at your fingertips
Workspace
Development workspace
nanoDDSCAT
Calculate scattering and absorption of light by targets with arbitrary geometries and complex refractive index.
Crystal Viewer Tool
Visualize different crystal lattices and planes
MOSFet
Simulates the current-voltage characteristics for bulk, SOI, and double-gate Field Effect Transistors (FETs)
High Impact Technology Exchange Conference
HI TEC
July 25–28, 2022
Grand America Hotel
Salt Lake City, UT

NanoDDSCAT

Calculate scattering and absorption of light with arbitrary geometry and complex Refractive Index

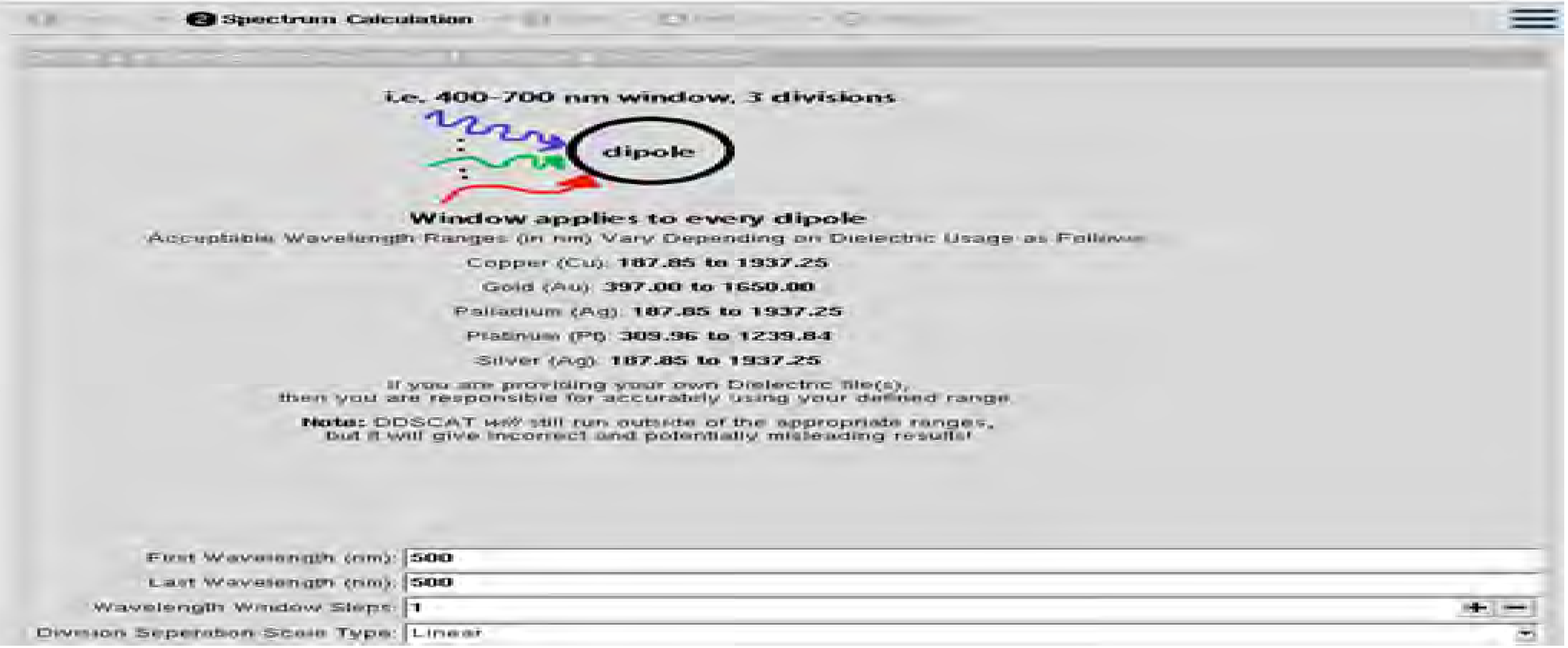
1. Target



NanoDDSCAT

Calculate scattering and absorption of light with arbitrary geometry and complex Refractive Index

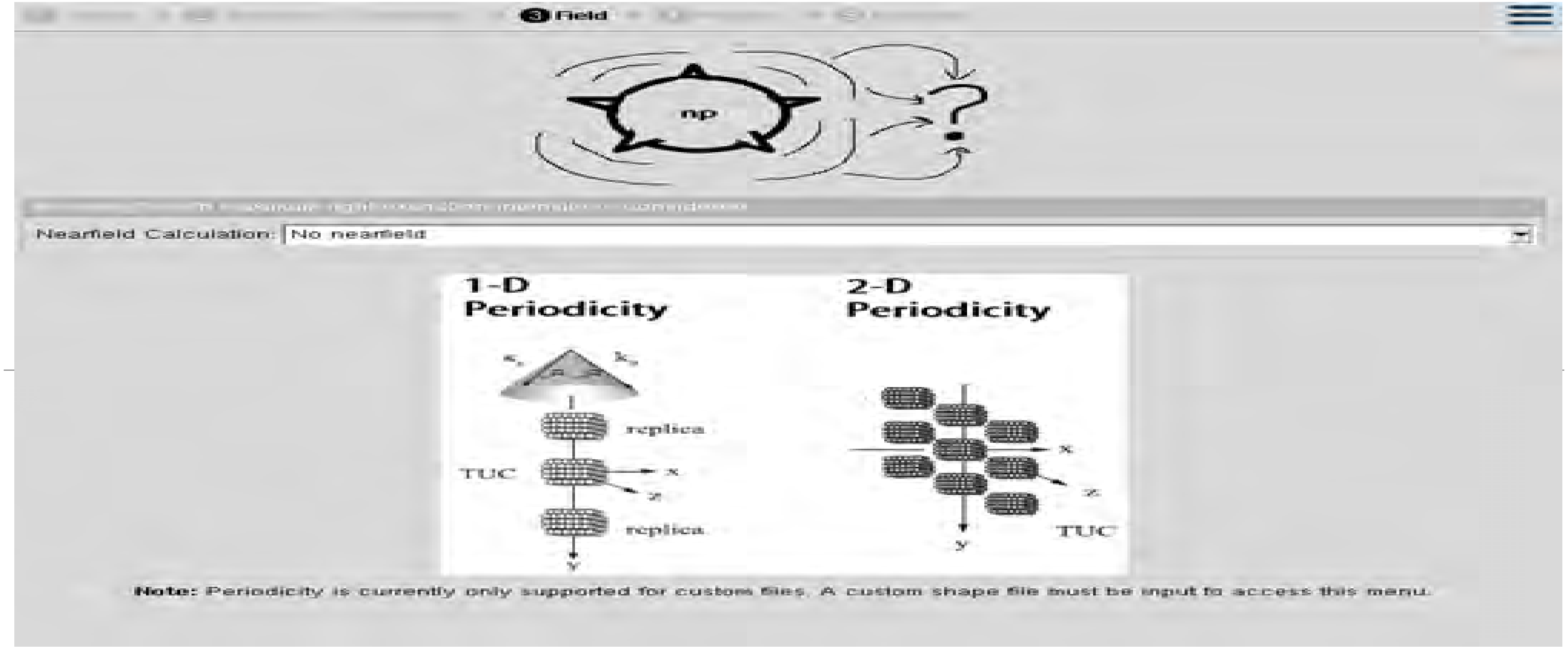
2. Spectrum Calculation



NanoDDSCAT

Calculate scattering and absorption of light with arbitrary geometry and complex Refractive Index

3. Field



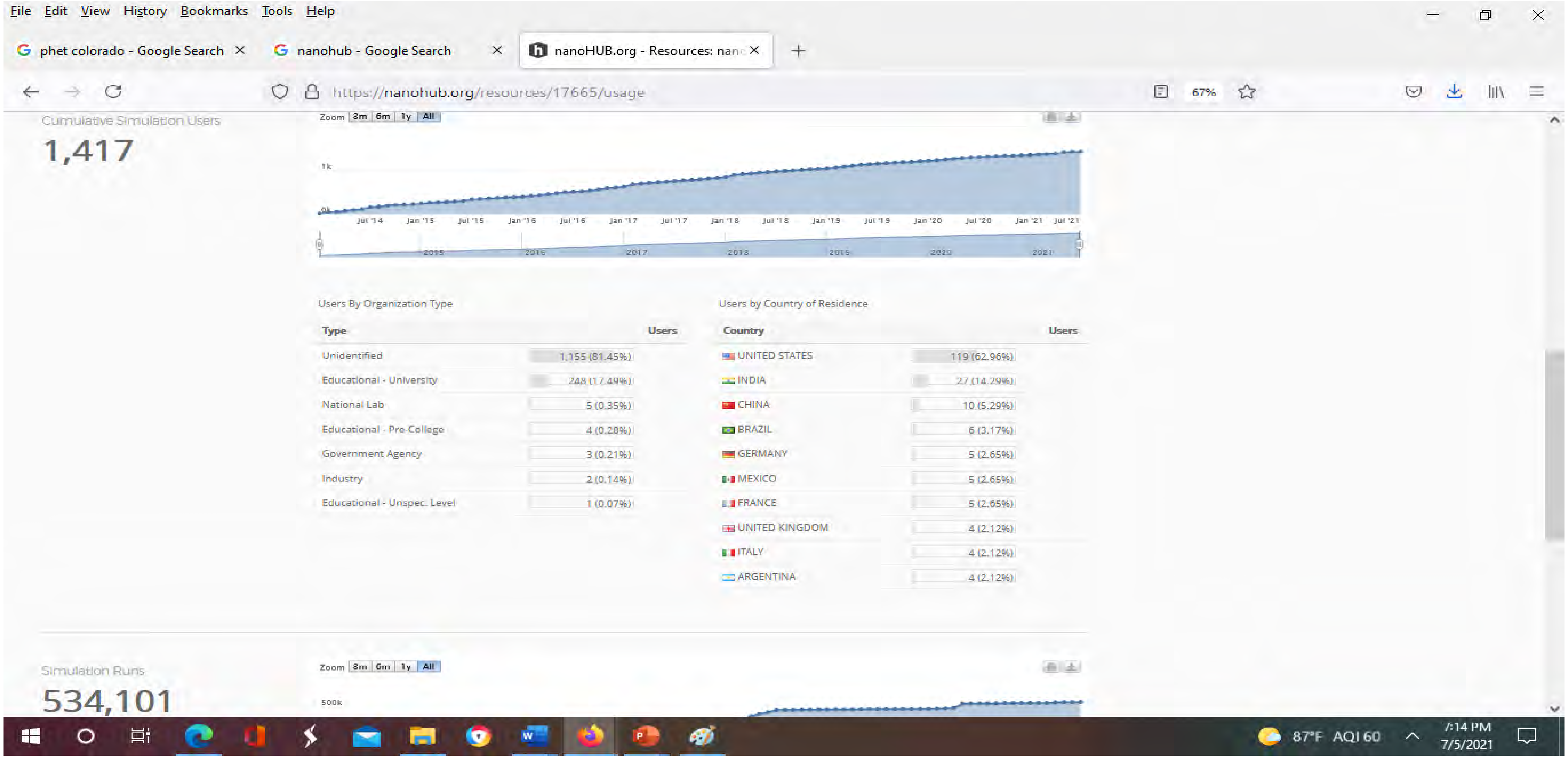
NanoDDSCAT

Calculate scattering and absorption of light with arbitrary geometry and complex Refractive Index

4. Process and Simulate

NanoDDSCAT

Worldwide Usage



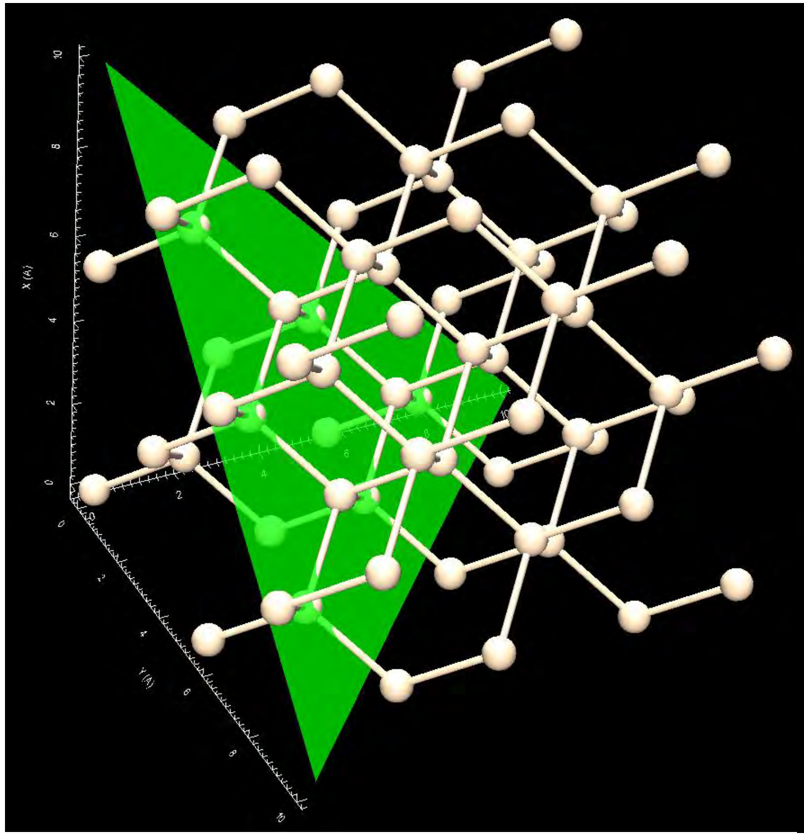
Users By Organization Type

Type	Users
Unidentified	1,155 (81.45%)
Educational - University	248 (17.49%)
National Lab	5 (0.35%)
Educational - Pre-College	4 (0.28%)
Government Agency	3 (0.21%)
Industry	2 (0.14%)
Educational - Unspec. Level	1 (0.07%)

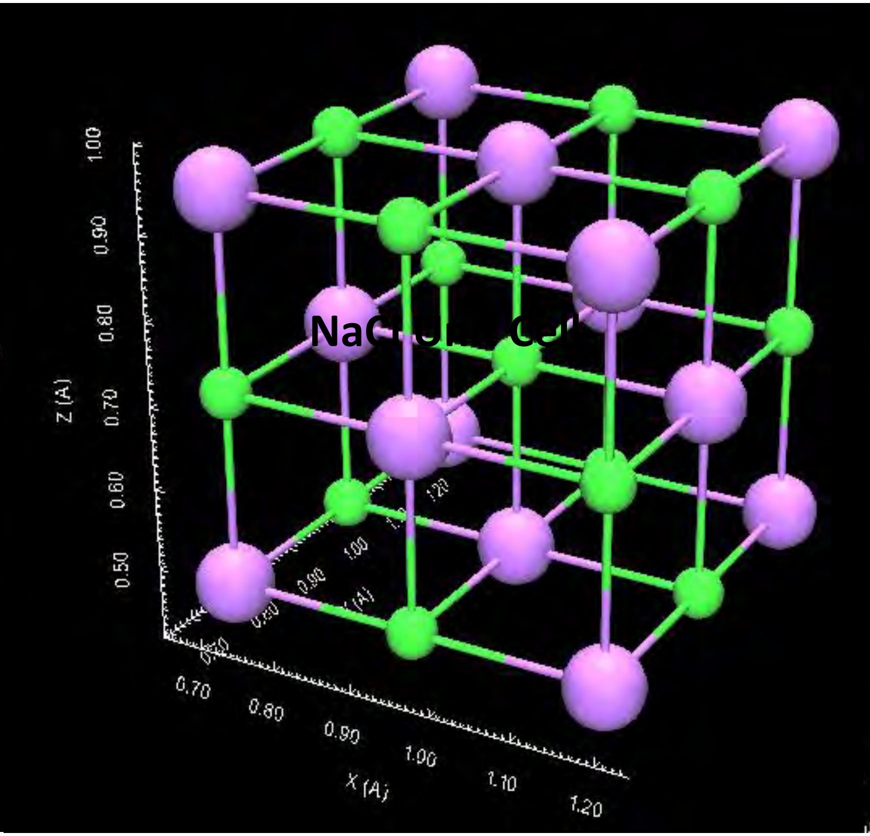
Users by Country of Residence

Country	Users
UNITED STATES	119 (62.96%)
INDIA	27 (14.29%)
CHINA	10 (5.29%)
BRAZIL	6 (3.17%)
GERMANY	5 (2.65%)
MEXICO	5 (2.65%)
FRANCE	5 (2.65%)
UNITED KINGDOM	4 (2.12%)
ITALY	4 (2.12%)
ARGENTINA	4 (2.12%)

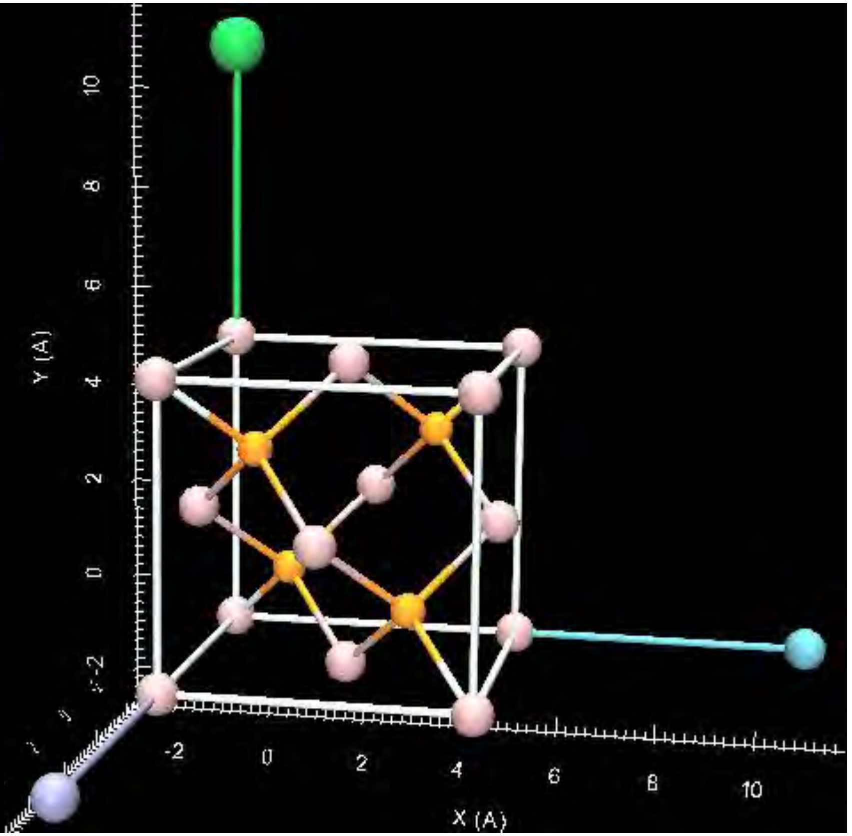
The Crystal Viewer simulation tool allows:
(a) viewing all materials which have periodical structure
(b) building crystal structure even not exists in nature



Silicon With Miller Plane

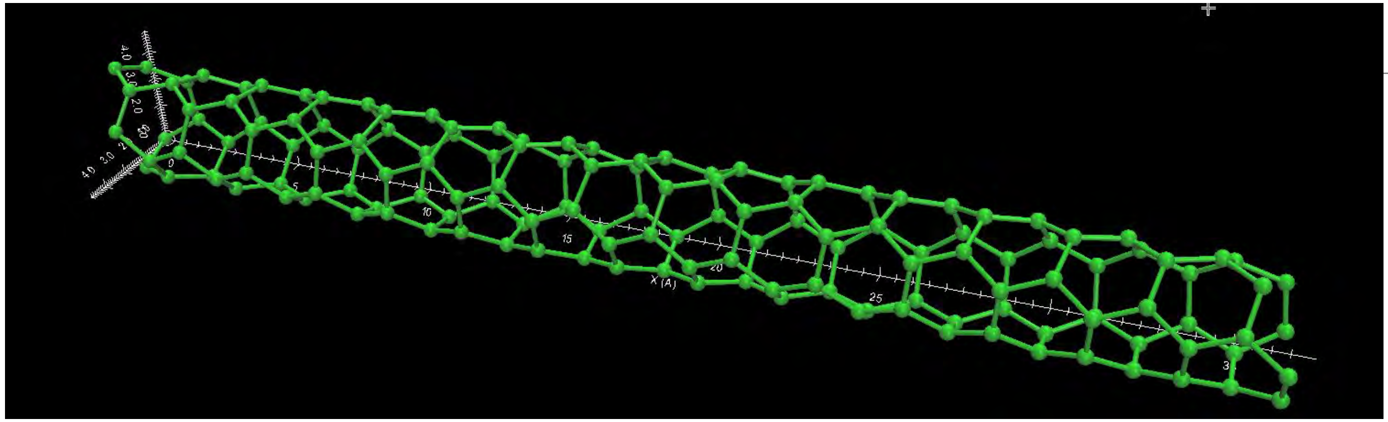


NaCl Unit Cell

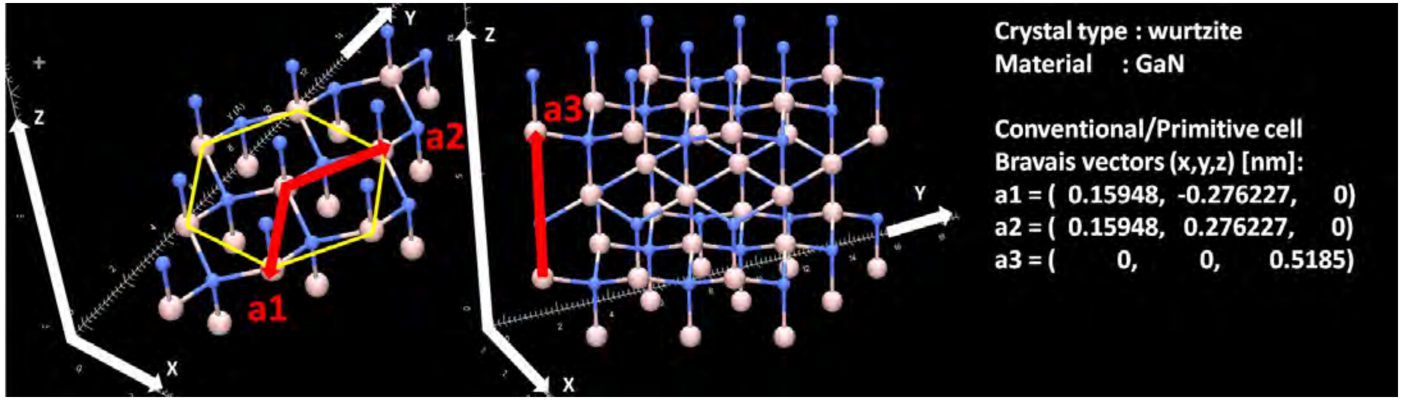


GaP Unit Cell

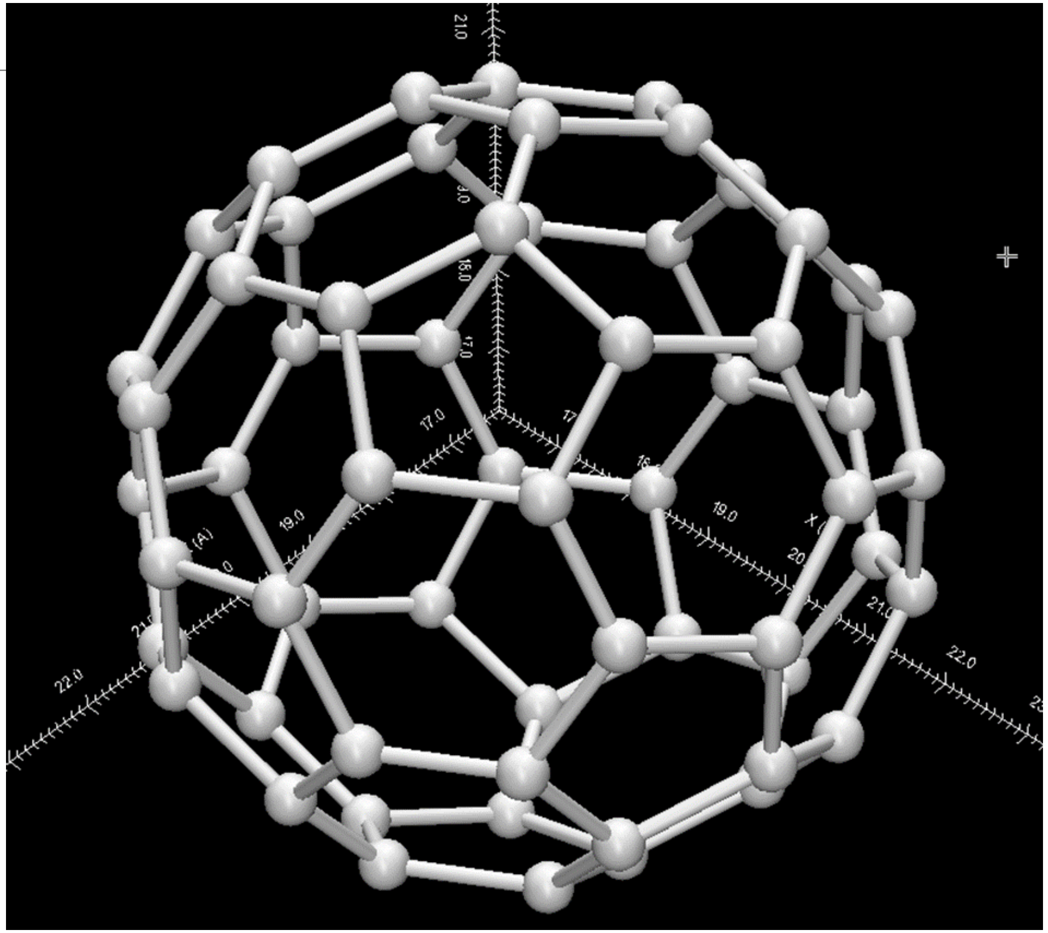
Examples of Nano Structure Visualization



Carbon nano tube



GaN Bravais Vectors



Buckey Ball

Crystal Viewer

Worldwide Usage

nanoHUB

RESOURCES EXPLORE NANOHUB-U PARTNERS COMMUNITY ABOUT SUPPORT DONATE TAKE A POLL

Cumulative Simulation Users

15,000

Users By Organization Type

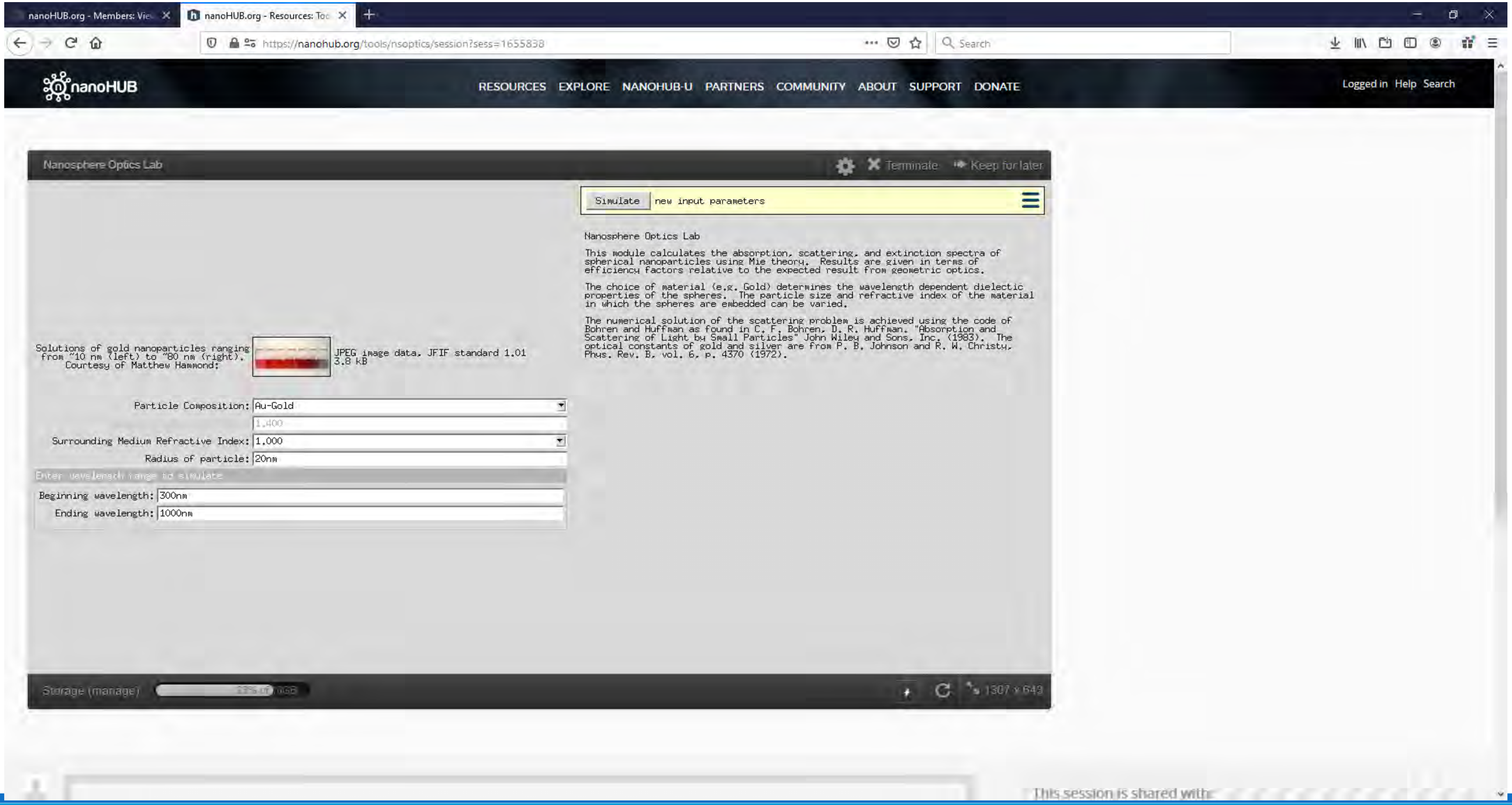
Type	Users
Unidentified	9,669 (64.43%)
Educational - University	4,890 (32.59%)
Industry	182 (1.21%)
National Lab	105 (0.7%)
Educational - Pre-College	59 (0.39%)
Unemployed	51 (0.34%)
Government Agency	41 (0.27%)
Military	9 (0.06%)

Users by Country of Residence

Country	Users
UNITED STATES	2,877 (67.82%)
INDIA	442 (10.42%)
PAKISTAN	305 (7.19%)
KOREA, REPUBLIC OF	119 (2.81%)
GERMANY	115 (2.71%)
COLOMBIA	84 (1.98%)
CHINA	82 (1.93%)
FRANCE	74 (1.74%)
UNITED KINGDOM	72 (1.7%)
CANADA	72 (1.7%)

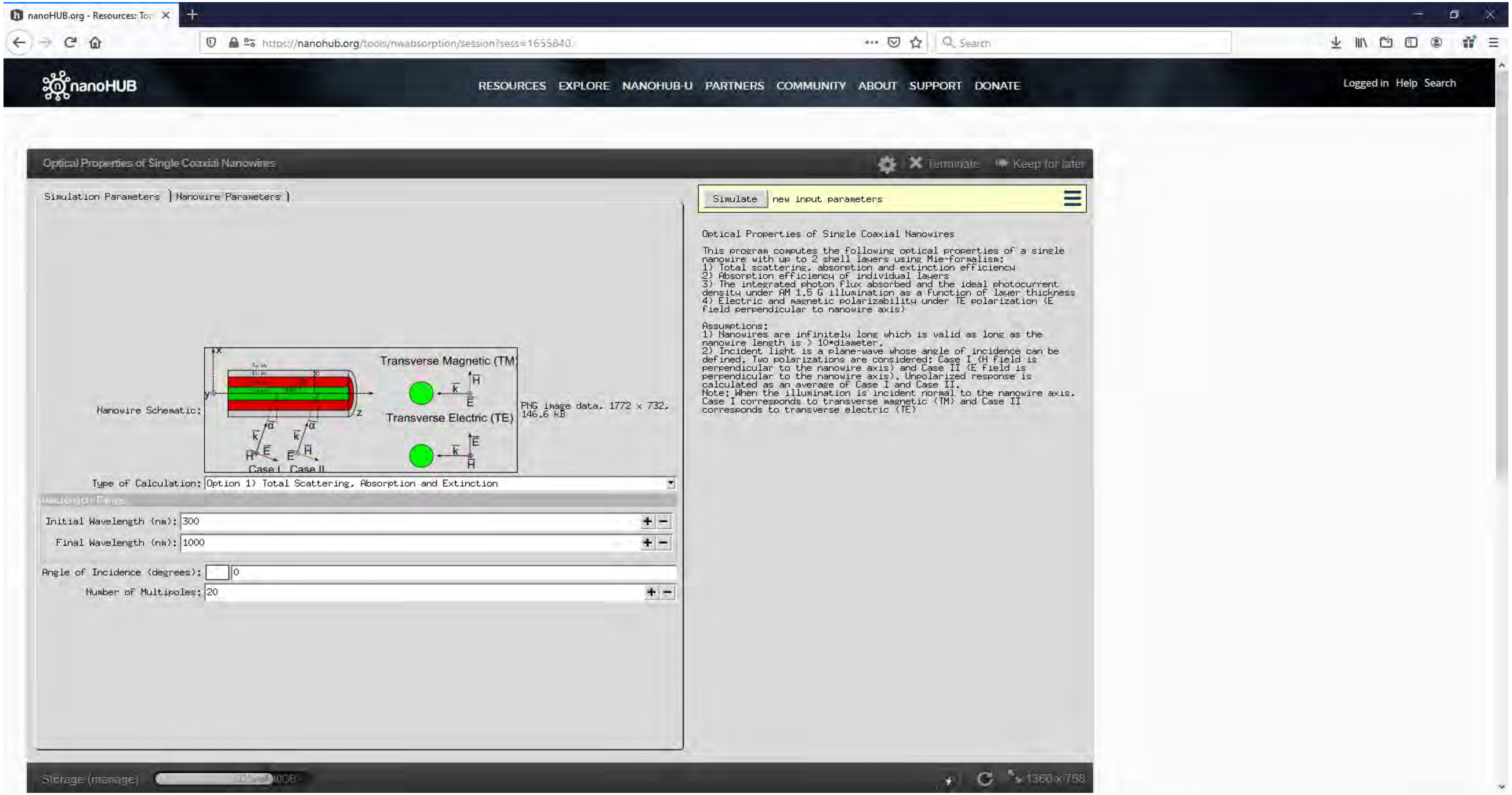
Nanosphere Optics Lab over NanoHub

Calculate absorption from metallic nanoparticles

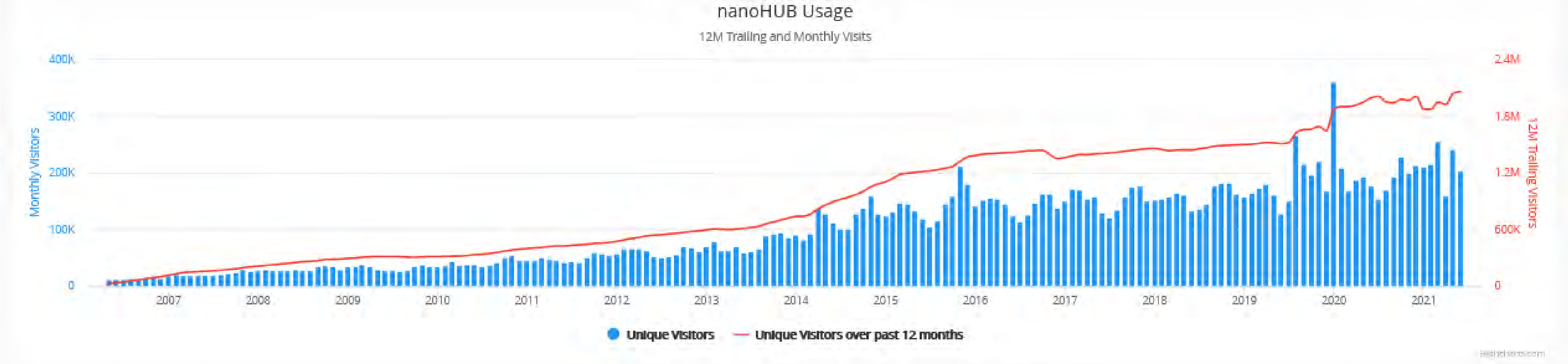


Nanosphere Optics Lab over NanoHub

Calculate absorption and scattering from single nanowires with or without shells



NanoHub:
Worldwide Usage



2,059,461 Unique Visitors	227,158 Registered Users	7,186 Resources	709 Published Tools

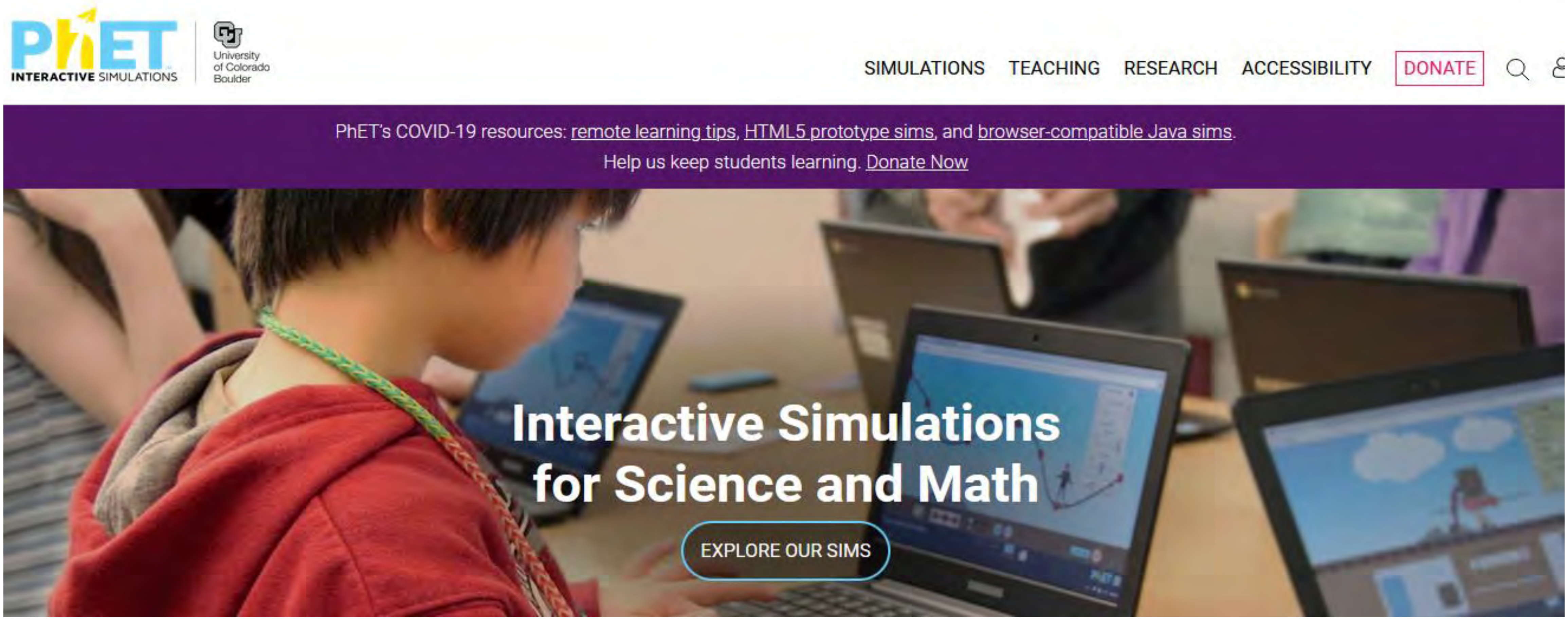
2,517 Citations	22,581 Simulation User Count

PhET Interactive Simulations

University of Colorado

For Physics, Chemistry, Math, Environmental Sciences and Biological Sciences:

https://phet.colorado.edu/



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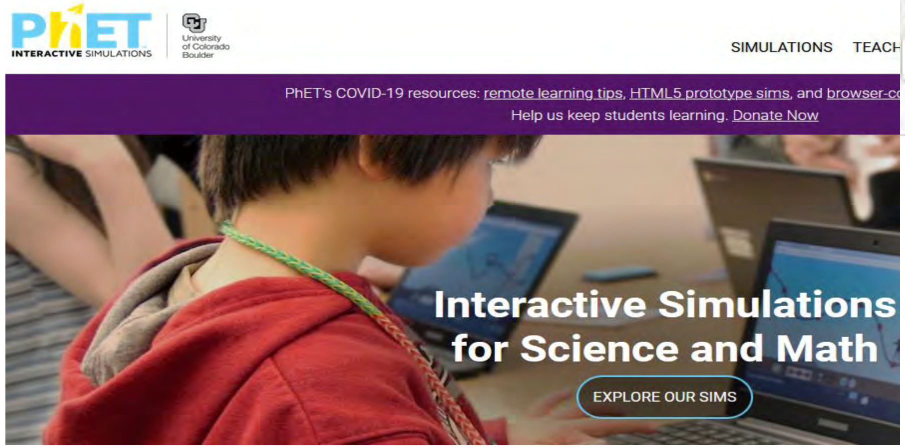
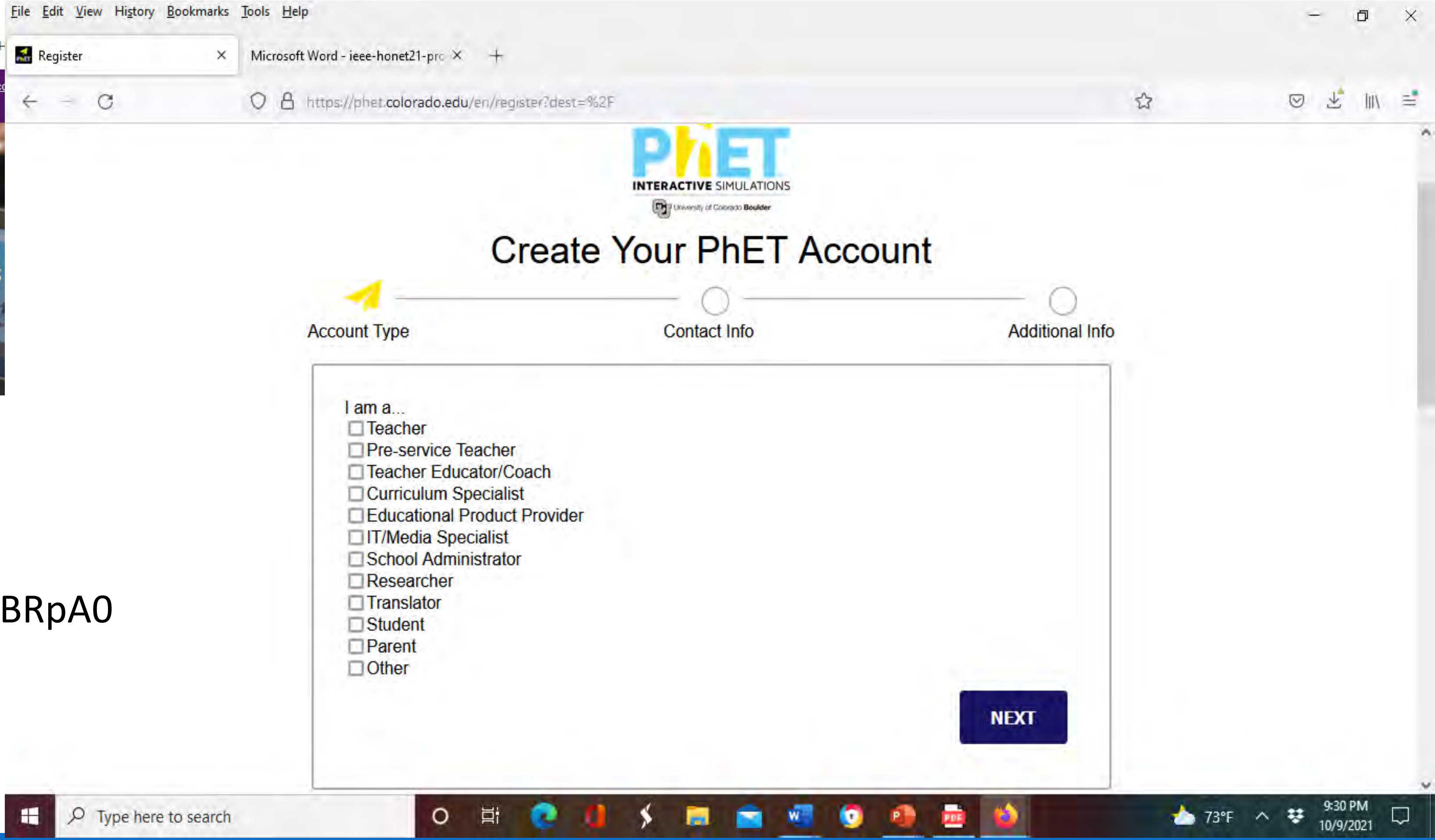




https://www.youtube.com/watch?v=4Hj6GqBRpA0

PhET Interactive Simulations

University of Colorado

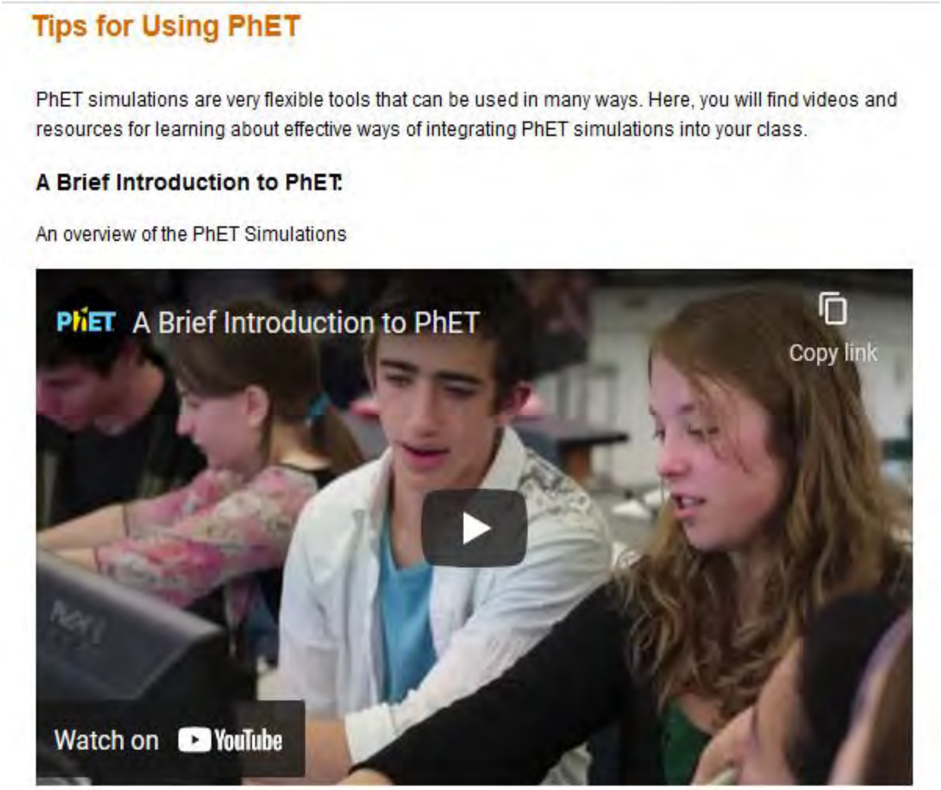
For Physics, Chemistry, Math, Environmental Sciences and Biological Sciences:
https://phet.colorado.edu/

PhET Simulations Help Students to:

- Engage in scientific exploration with multiple, positive learning
- Achieve conceptual learning
- Make connections to everyday life (e.g., science to the real world)
- Take and sense ownership of their learning

PhET Simulations Help Educators to:

- Create a student-centered classroom
- Foster a supportive, goal-oriented learning environment
- Bring their experience, professionalism, and knowledge of their students to designing, implementing, and improving activities, implementation, and design.



PhET Interactive Simulations: Accessibility Features

University of Colorado

For Physics, Chemistry, Math, Environmental Sciences and Biological Sciences:

https://phet.colorado.edu/

INTERACT
DISCOVER
LEARN

160 interactive simulations	95 language translations	2980 teacher-submitted lessons

Accessible Simulations

▼ Accessibility Features

- Alternative Input (e.g., keyboard navigation) ⊞
- Sound and Sonification ⊞
- Interactive Description ⊞
- Interactive Description on Mobile Devices ⊞
- Pan and Zoom ⊞
- Voicing ⊞

https://www.youtube.com/watch?v=4Hj6GqBRpA0

PhET Interactive Simulations: Sample Simulations

For Physics, Chemistry, Math, Environmental Sciences and Biological Sciences:
https://phet.colorado.edu/

Balloons and Static Electricity

- Published Version: Balloons and Static Electricity
- Grab a balloon to explore concepts of static electricity such as charge transfer, attraction, repulsion, and induced charge.

Coulomb's Law

- Published Version: Coulomb's Law
- Observe changes to electrostatic force as you play with the distance between charges and charge amounts at both macro and atomic scales.

Faraday's Law

- Published Version: Faraday's Law
- Investigate Faraday's law and how a changing magnetic flux can produce a flow of electricity!

Friction

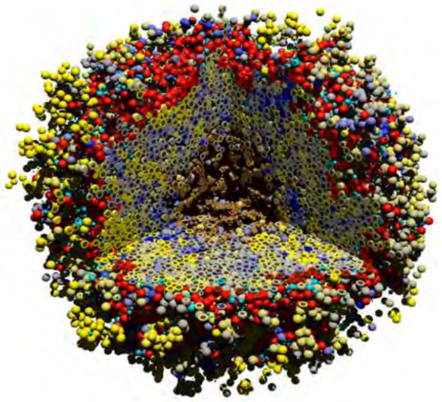
- Published Version: Friction

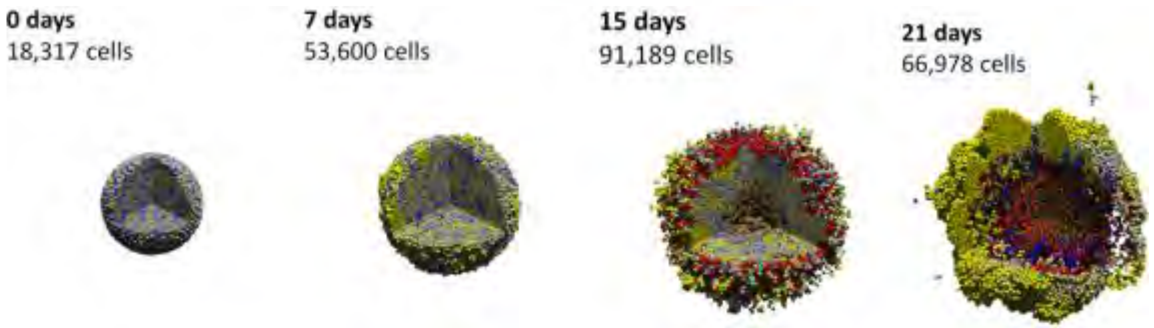
A complete list is available at: https://phet.colorado.edu/en/accessibility/prototypes

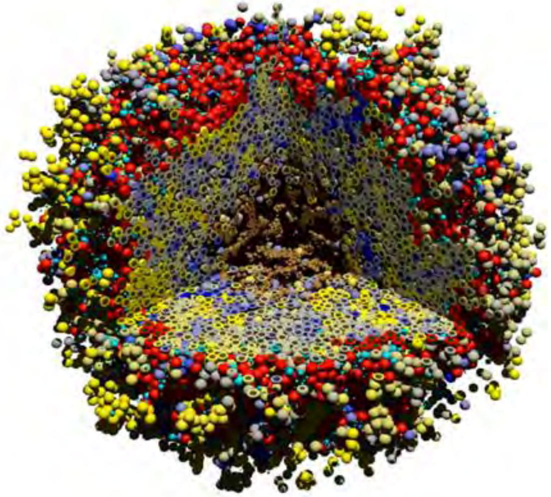
PhysiCell provides a robust, scalable code for simulating large systems of cells in 3-D tissues on standard desktop computers
http://physicell.org/

PhysiCell

ABOUT | LEARN | ECOSYSTEM | DOWNLOADS | NEWS | COMMUNITY | CONTACT







An open source physics-based cell simulator

http://physicell.org/

Physicell can also be accessed via nanoHub.

PhysiCell

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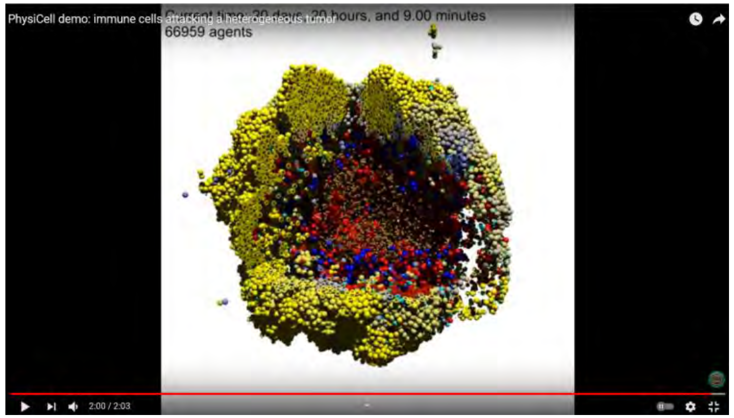
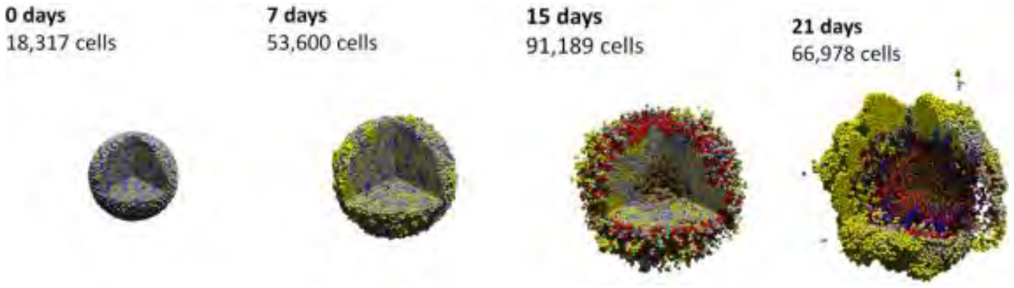
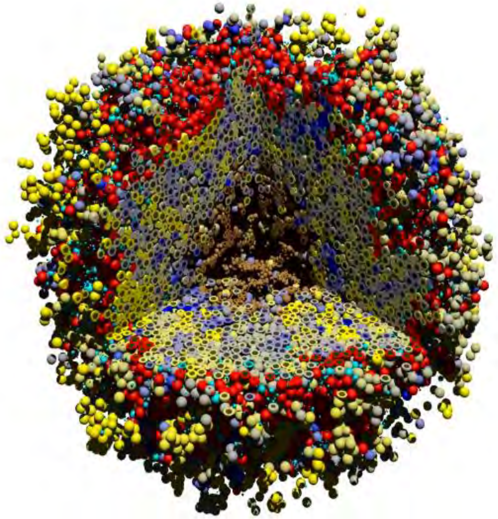
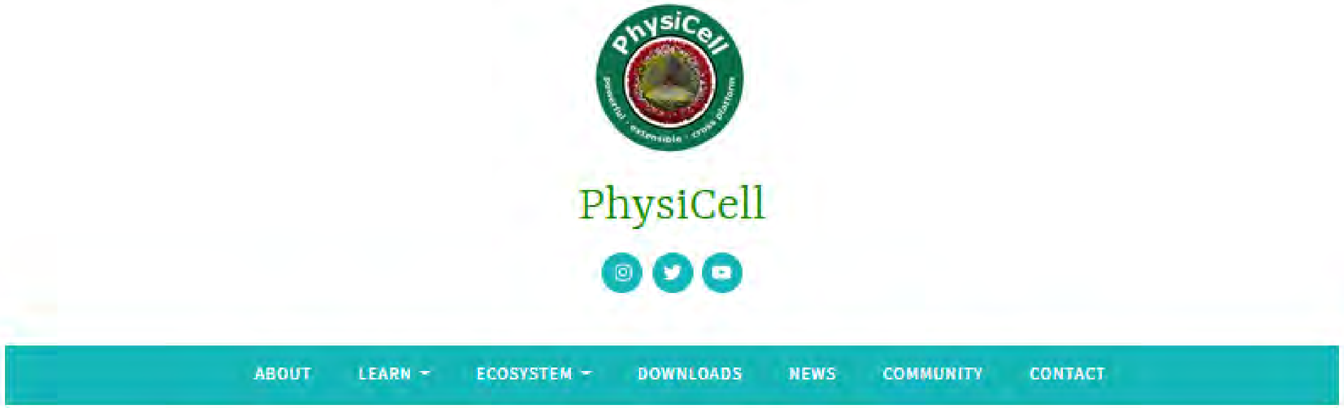


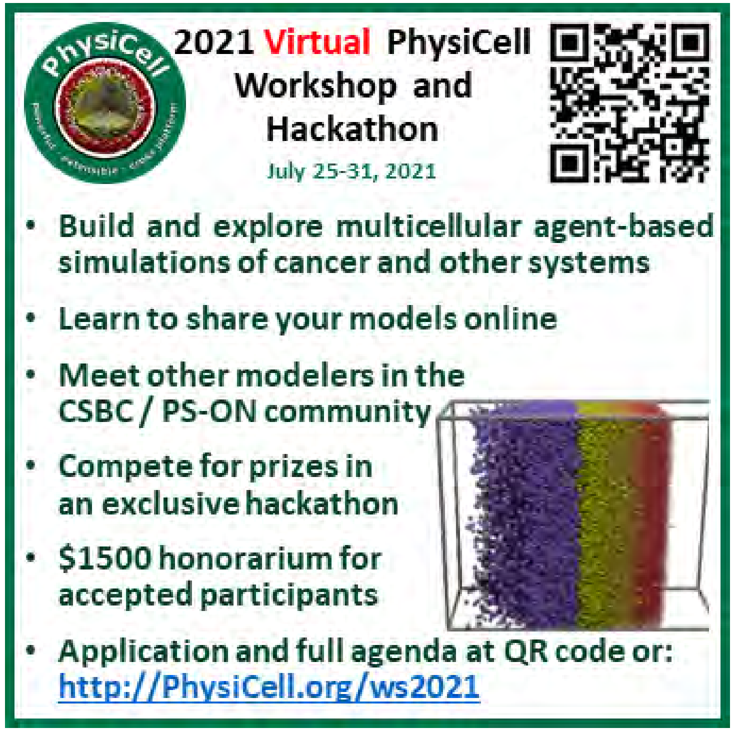


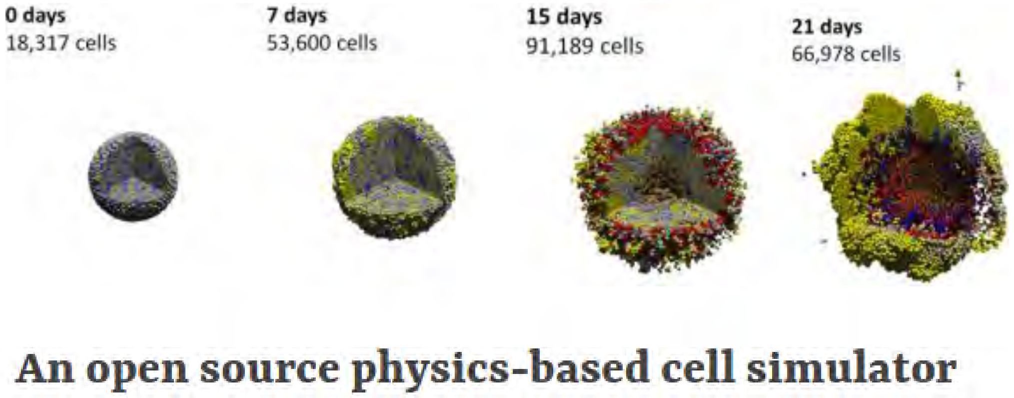
An open source physics-based cell simulator



[PhysiCell demo: immune cells attacking a heterogeneous tumor](https://youtu.be/nJ2urSm4ilU)
https://youtu.be/nJ2urSm4ilU







COVID19 tissue simulator

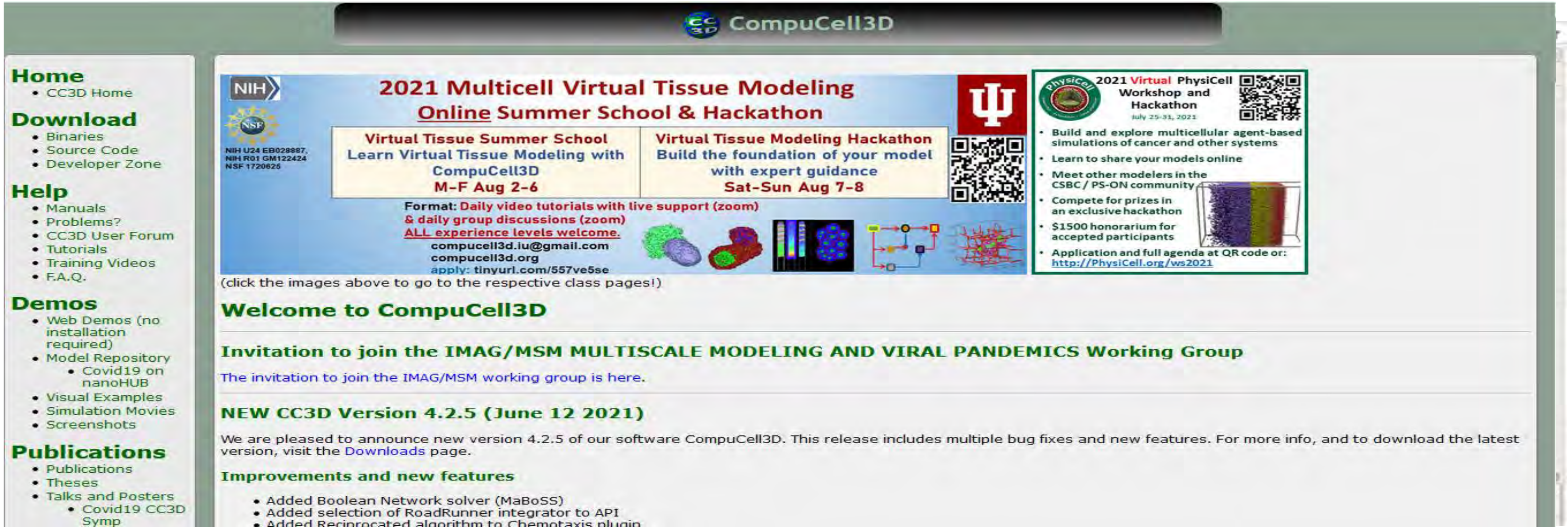
This model simulates viral dynamics of SARS-CoV-2 (coronavirus / COVID19) in a layer of epithelium and several submodels (such as single-cell response, pyroptosis death model, tissue-damage model, lymph node model and immune response).

http://physicell.org/

Physicell can also be accessed via nanoHub.

CompuCell3D

CompuCell3D is a flexible scriptable modeling environment, which allows the rapid construction of sharable Virtual Tissue in-silico simulations of a wide variety of multi-scale, multi-cellular problems including angiogenesis, bacterial colonies, cancer, developmental biology, evolution, the immune system, tissue engineering, toxicology and even non-cellular soft materials. CompuCell3D models have been used to solve basic biological problems, to develop medical therapies, to assess modes of action of toxicants and to design engineered tissues. CompuCell3D intuitive and make Virtual Tissue modeling accessible to users without extensive software development or programming experience. It uses Cellular Potts Model to model cell behavior.



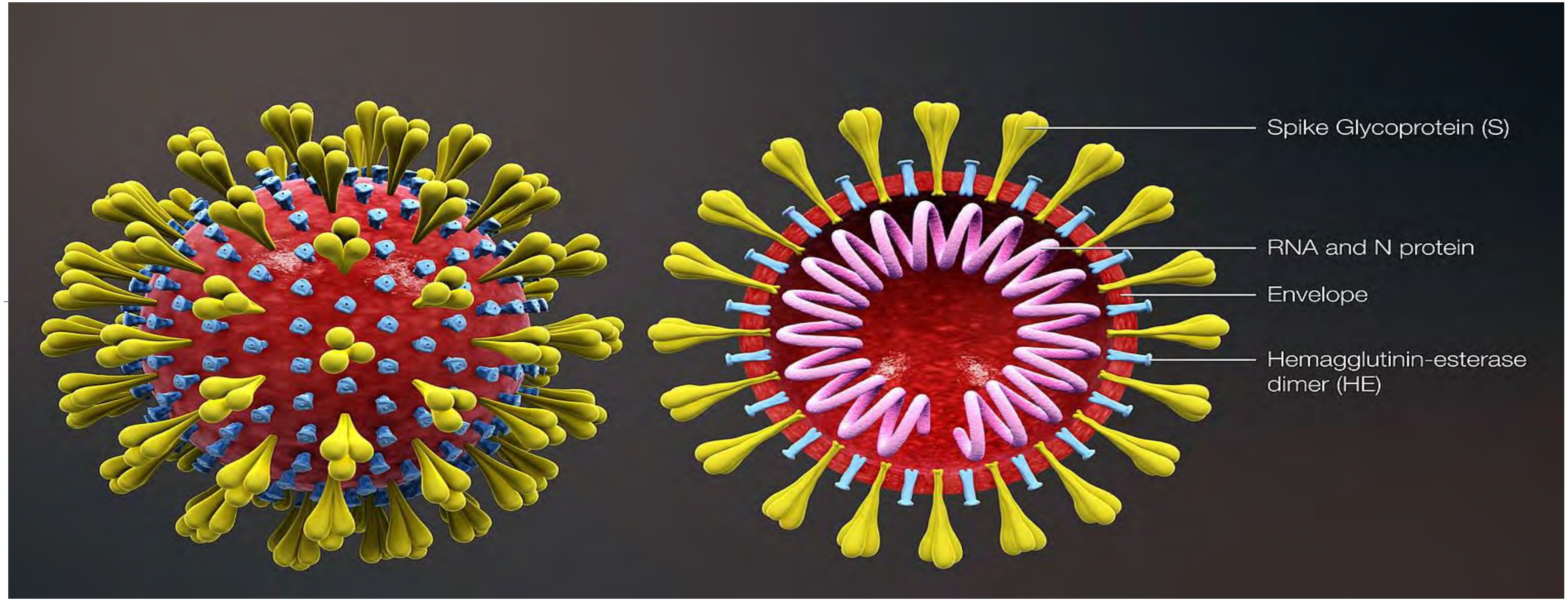
Example of the Application of CompuCell3D

A multiscale model of viral infection in epithelial tissues

COVID 19 Virtual Tissue Model - Tissue Infection and Immune Response Dynamics

By Josua Oscar Aponte-Serrano, T.J. Sego

Simulates tissue and immune system interactions during a viral lung infection



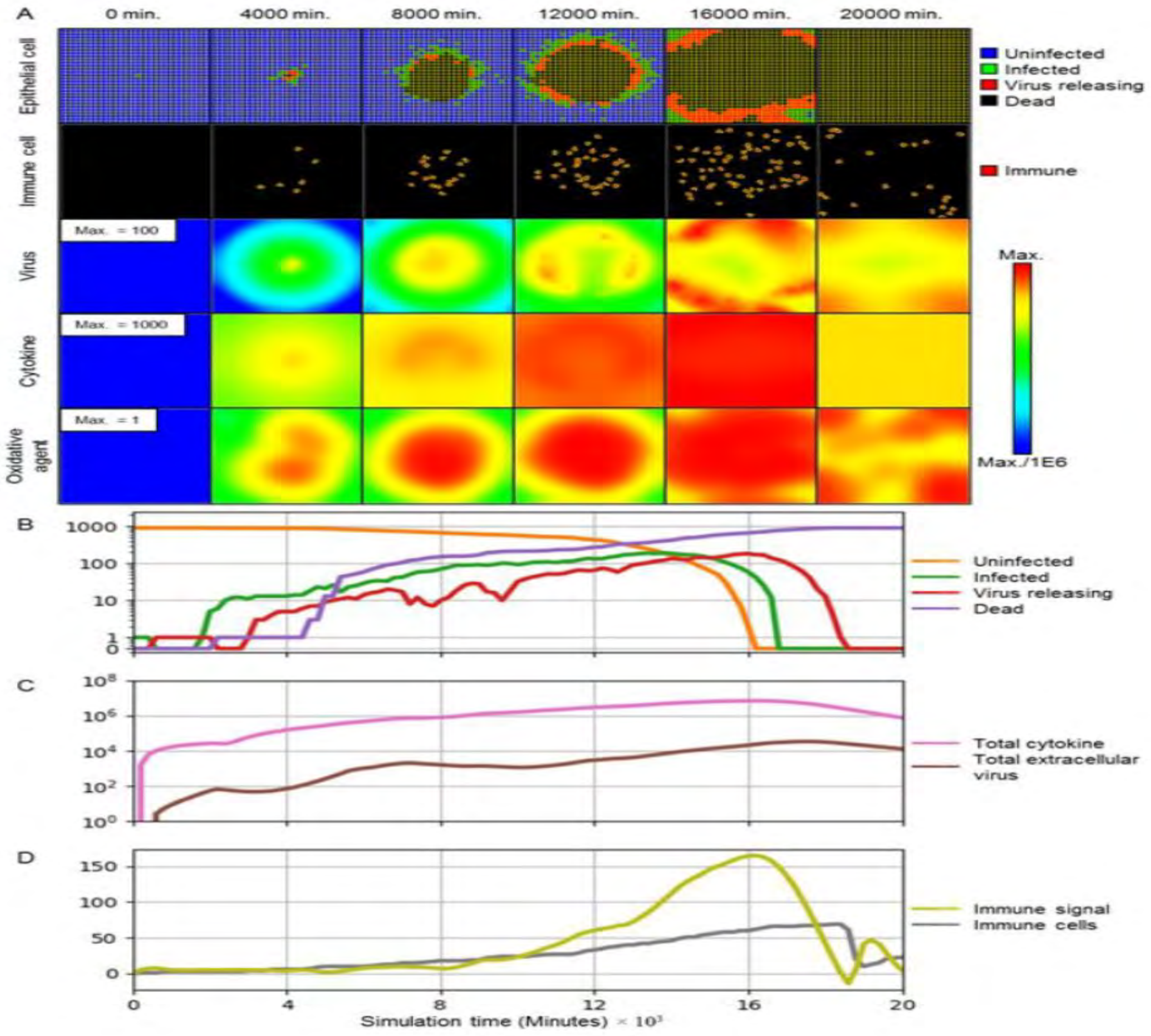


Figure 3. Simulation of the progression of infection in a patch of epithelial tissue of size 360 μm x 360 μm starting from a single infected cell for a representative simulation using the baseline parameters given in Table 1. A. Snapshots of spatial configuration *vs* time, showing progression of a simulated infection. Columns, left to right: 0 minutes (time of initial infection), 4000 minutes (67 hours, 2 ¾ days) after infection, 8000 minutes (133 hours, 5 ½ days), 12000 minutes (200 hours, 8 ⅓ days), 16000 minutes (267 hours, 11 days), and 20000 (333 hours,

Example of the Application of CompuCell3D

A modular framework for multiscale, multicellular, spatiotemporal modeling of acute primary viral infection and immune response in epithelial tissues and its application to drug therapy timing and effectiveness

A multiscale model of viral infection in epithelial tissues

T.J. Sego 1,2* , Josua O. Aponte-Serrano 1,2* , Juliano Ferrari Gianlupi 1,2 , Samuel R. Heaps 1 , Kira Breithaupt 1,3 , Lutz Brusch 4 , James M. Osborne 5 , Ellen M. Quardokus 1 , Richard K. Plemper 6 , James A. Glazier 1,2

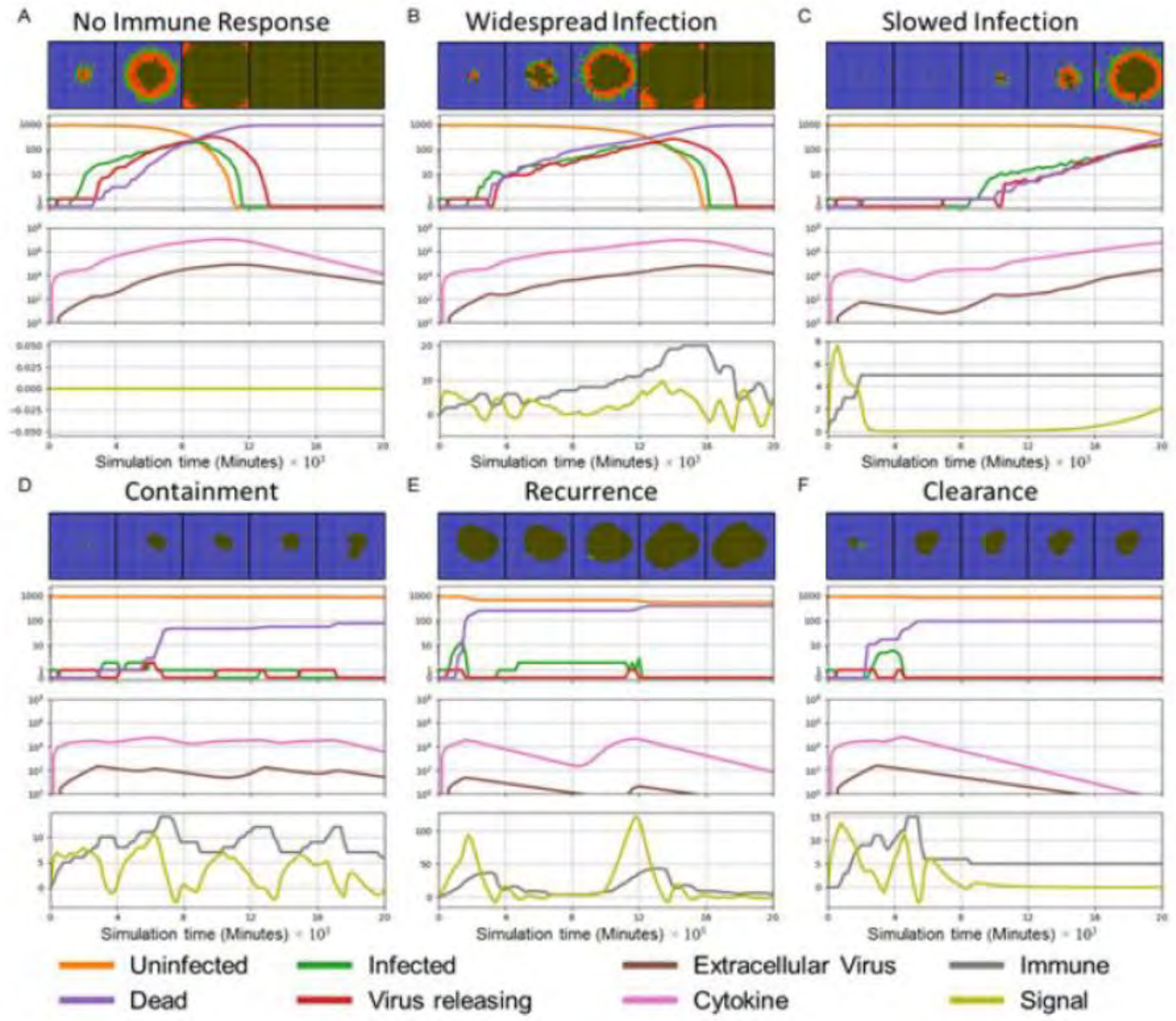


Figure 4. Patterns (classes) of spatiotemporal infection dynamics. First row: snapshots of spatial configurations of the epithelial cells. Color coded: uninfected (blue), infected (green), virus releasing (red), dead (black). Times from

Example of the Application of CompuCell3D

A multiscale model of viral infection in epithelial tissues

A modular framework for multiscale, multicellular, spatiotemporal modeling of acute primary viral infection and immune response in epithelial tissues and its application to drug therapy timing and effectiveness

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CompuCell3D Multiscale, Virtual-Tissue Spatio-Temporal Modeling of Simulations of COVID-19 Infection, Viral Spread and Immune Response and Treatment Regimes

"Simulations of tissue-specific effects of primary acute viral infections like COVID-19 are essential for understanding differences in disease outcomes and optimizing therapeutic interventions. In this two-part mini-workshop we present an open-source Python and CC3DML-scripted multiscale model and simulation of an epithelial tissue infected by a virus, a simplified cellular immune response and viral and immune-induced tissue damage and show how you can use it to model basic patterns of infection dynamics and antiviral treatment. Part I presents the model and teaches how to run it and to change model parameters for generating new biologically meaningful simulations. Part II teaches how to extend the model with additional images, graphics and file outputs, additional cell types, diffusive fields, cell behaviors and interactions and improved subcellular and immune-system models." [https://compucell3d.org/]

How to Run, Extend, Adapt and Improve the CompuCell3D COVID-19 Model

Part-I: Video

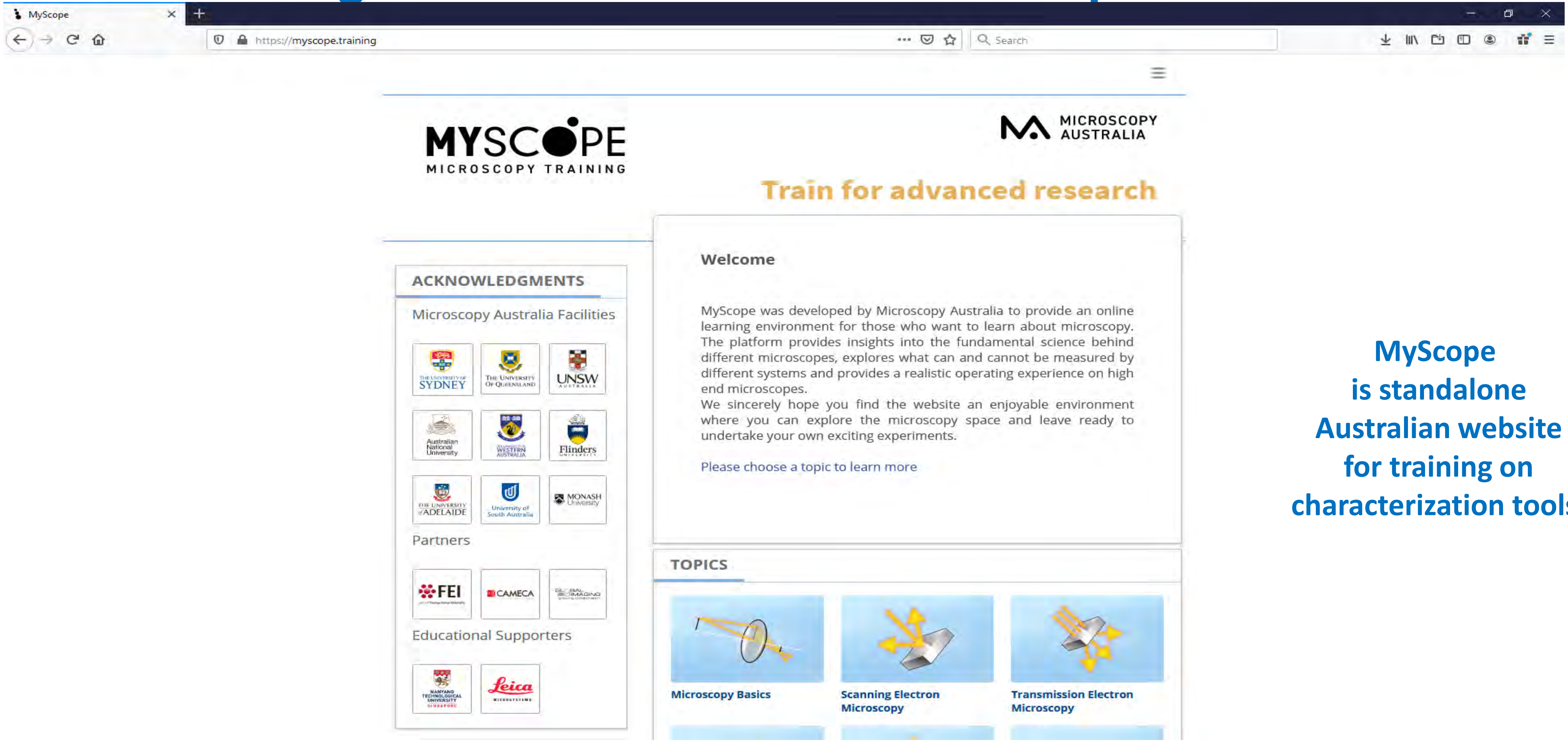
https://www.youtube.com/watch?v=edL8yHE8cO8&feature=youtu.be

Part-II: Video

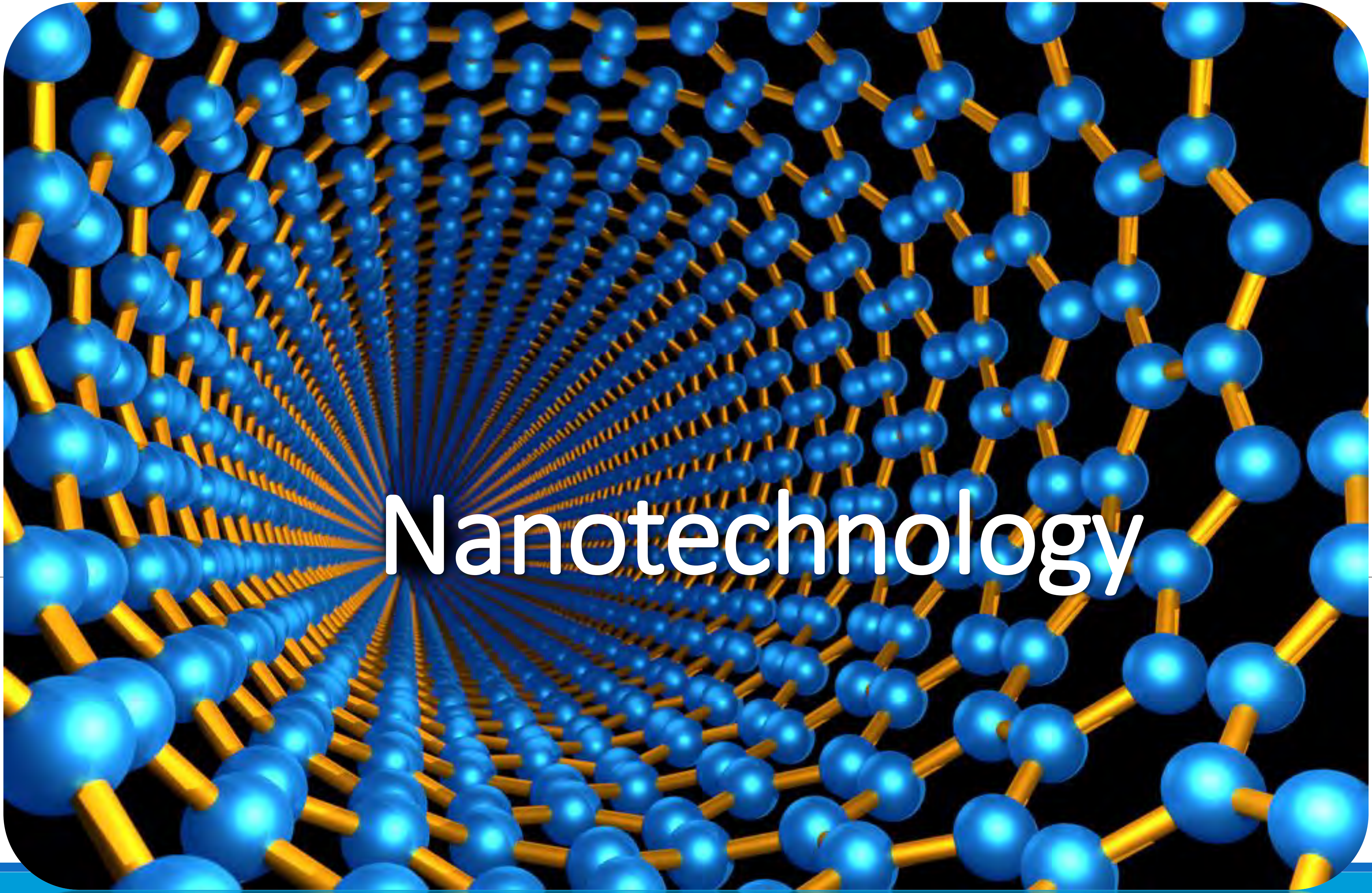
https://www.youtube.com/watch?v=hDc0ttw_wqo&feature=youtu.be

CompuCell3D can be downloaded from https://compucell3d.org/SrcBin or it could be accessed via NanoHub.

Another Online Resource:
A great characterization virtual experience:



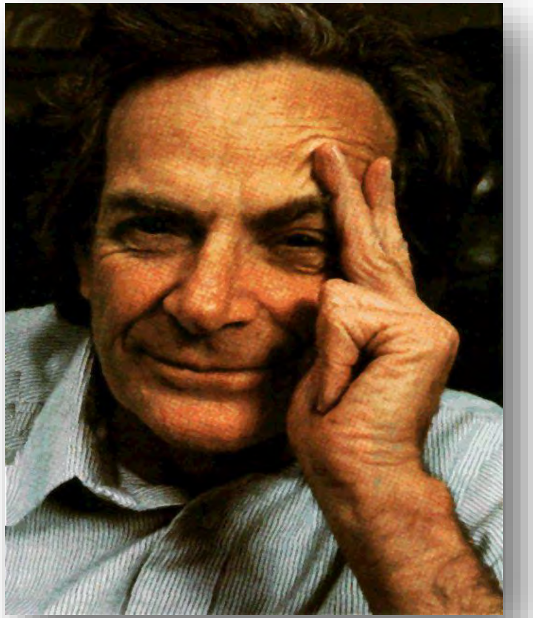
MyScope is standalone Australian website for training on characterization tools.



Nanotechnology

Nanotechnology

The term “nanotechnology” covers processes associated with the creation and utilization of structures in the 1 nanometer (nm) to 100 nm range.
It refers to the ability to design, investigate, modify, model, or manipulate any substance at the molecular or atomic level (nanometer scale).
Nanometer = 1 billionth of a meter (100 thousand time smaller than human hair) or 10 hydrogen atoms in a line.



Richard P. Feynman
(1918 - 1988, Nobel 1965)

Although nanotechnology existed in the prehistoric time, the concept underlying nanotechnology was first discussed by Richard Feynman in 1959

There’s Plenty of Room at the Bottom- Feynman
“The principles of physics, as far as I can see, do not speak against the possibility of maneuvering things atom by atom.”
“The problems of chemistry and biology can be greatly helped if our ability to see what we are doing, and to do things on an atomic level, is ultimately developed...”

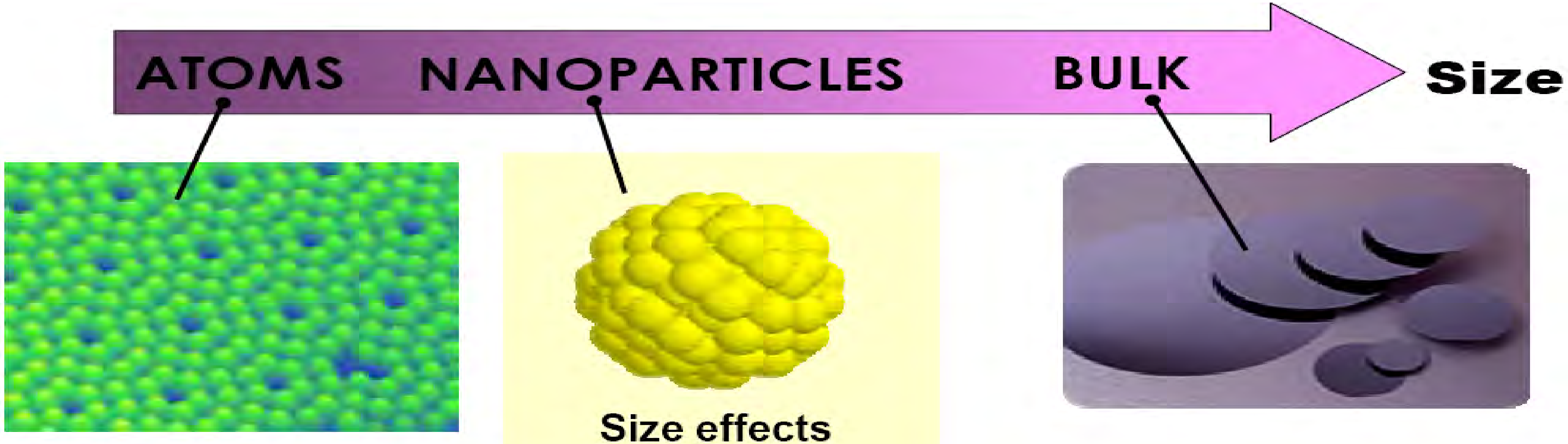
Examples of Nanoscale phenomena

Matter appearing in the form of solids, liquids and gases can exhibit unusual physical, Chemical and biological properties at the nanoscale, differing In important ways from the properties of bulk materials. The boundaries between traditional disciplines of science such as biology, chemistry and
Physics disappear when characterizing or describing the behavior of matter at the nanoscale

For example:
•Bulk gold appears yellow in color but 12nm(nanosized)gold particles appear red.
•largeZnO(zincoxide)particles(traditionalsunscreen)scatter visible light and appear white but nanosized ZnO particles of 30nm do not scatter light and appear transparent.

Promise of Nanotechnology

- Better understanding of nature and life
- Environmental benefits for energy, water supply, and agriculture
- Likelihood of extending life and improving health
- Host of new products that could in the next 10-15 years have a value of $1 trillion a year



Size effects

↓

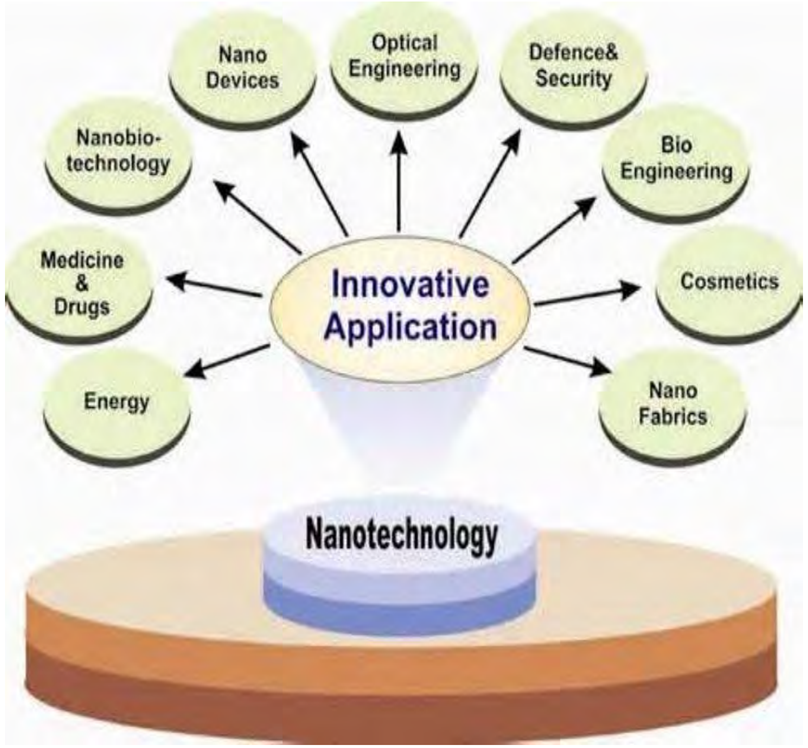
Electronic and vibrational states and transitions show deviations from those in the bulk.

↓

Tunable new properties!!!

Most promising beneficiaries (not ranked in any manner) of nanotechnology application.

- Electronics and Semiconductors
– Information Technology (Computing and Telecommunication)
- Aerospace and Automotive Industries
- Chemical Processes and Engineering
– Agriculture - Energy - Disease Diagnosis
– Health Monitoring
- Drug Delivery
- Food Processing and Storage
- Water Treatment and Air Pollution Control



Everyday Applications

Due to their anti-microbial activities, silver nanoparticles have been incorporated into many consumer products including: In 2013. It listed 1814 consumer products. 435 used silver nanomaterial.

- Dietary supplements
- laundry detergents
- Body soap
- Toothbrushes
- Toothpaste
- Disinfectant sprays
- Kitchen utensils
- Clothing and children’s toys





Market Size

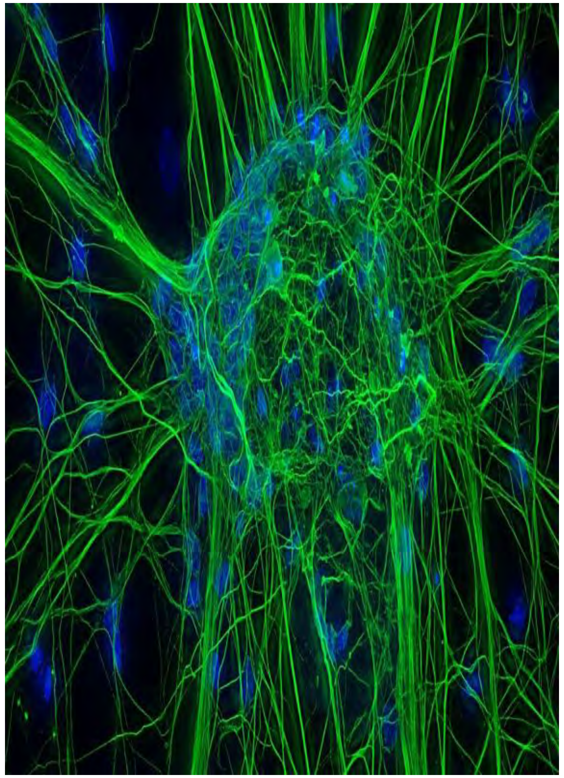
According to Emergen Research Nanotechnology Market Size, Share, Trends, By Type (Nanomaterials, Nanocomposites, Nano devices, Nano tools), By Industry (Food and Agriculture, Healthcare, Information and Technology, Environment, Energy, Cosmetics), and By Region, Forecast to reach USD 290.93 Billion in 2028.

https://www.globenewswire.com/en/newsrelease/2021/05/18/2231845/0/en/Nanotechnology-Market-Size-to-Reach-USD-290-93-Billion-in-2028-Advancements-in-Technology-and-Rising-Investment-in-Research-Development-by-Market-Players-is-Driving-Industry-Growth.html

Need For Visualization at the Nanoscale

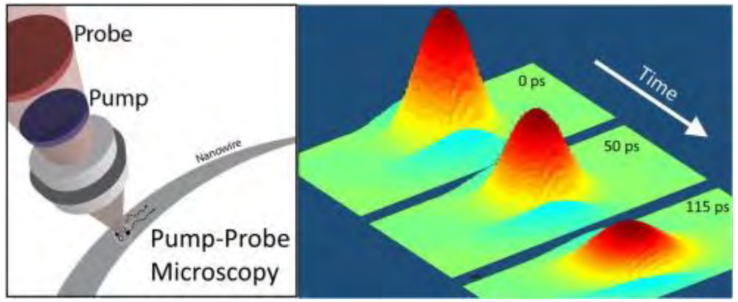
- Visualization of physical phenomena can confirm hypothesis
- Observation provides opportunities for study without damaging the sample.
- Objects under study may be too small for our hands to handle or manipulate
- Our students are motivated by “seeing for themselves”!
- Measurement tools for nanotechnology applications is expected to create a multibillion-dollar market within the next decade
- Morphologic characterization of Viruses such as Covid-19
- Development of new products based on nanotechnology requires visualization coupled with interfacial interactions, and measurement at the nanoscale.

THUNDER Imager 3D Live Cell & 3D Cell Culture - Decode 3D Biology in Real Time*



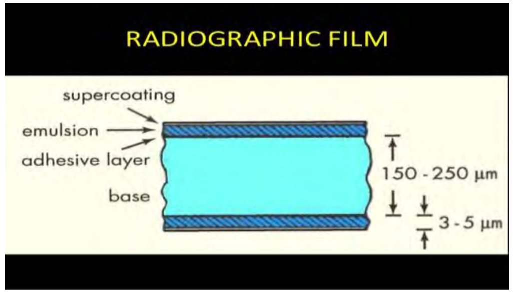
Advantages of Visualization at the Nanoscale

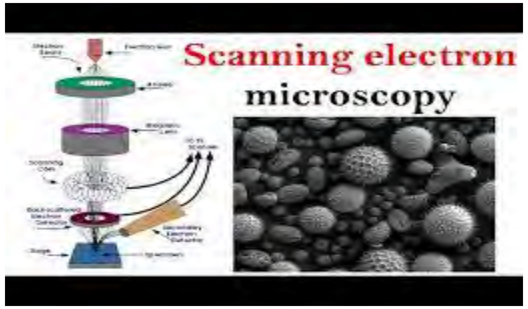
- Enhance students understanding of the properties of matter at the nanoscale which differ from bulk material.
- Help instructors improve teaching of abstract concepts of nanoscale phenomena.
- Understand the benefits and application of visualization at the nanoscale.
- Increase knowledge in the field of nanotechnology and STEM education.
- Understand the use of remotely accessible instruments for visualization of nanoscale samples .



Options in Visualization

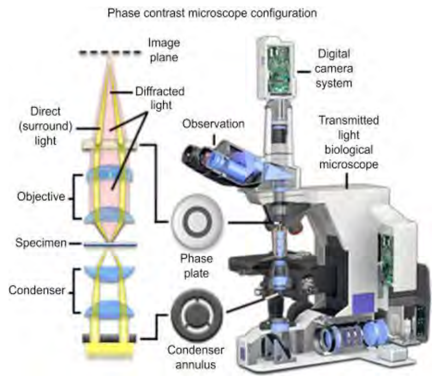
- Observe the sample with shorter wavelengths of light or radiation
  - Need to convert the imaging result into something that we can visualize
    - X-Ray film
    - Scanning Electron Microscope
- Probe the sample physically
  - Need to be very, very careful
    - Mechanical feedback
    - Motion to vision conversion required

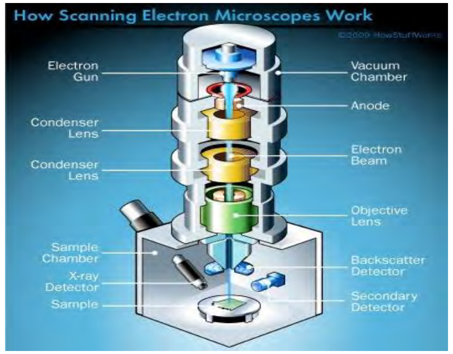


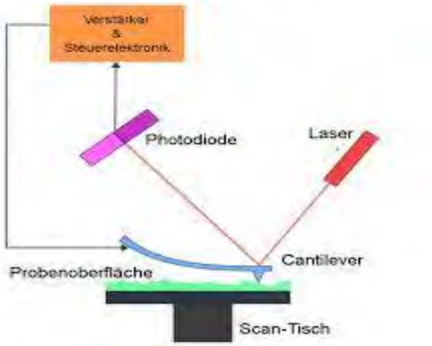


Methods of Nanoscale Visualization

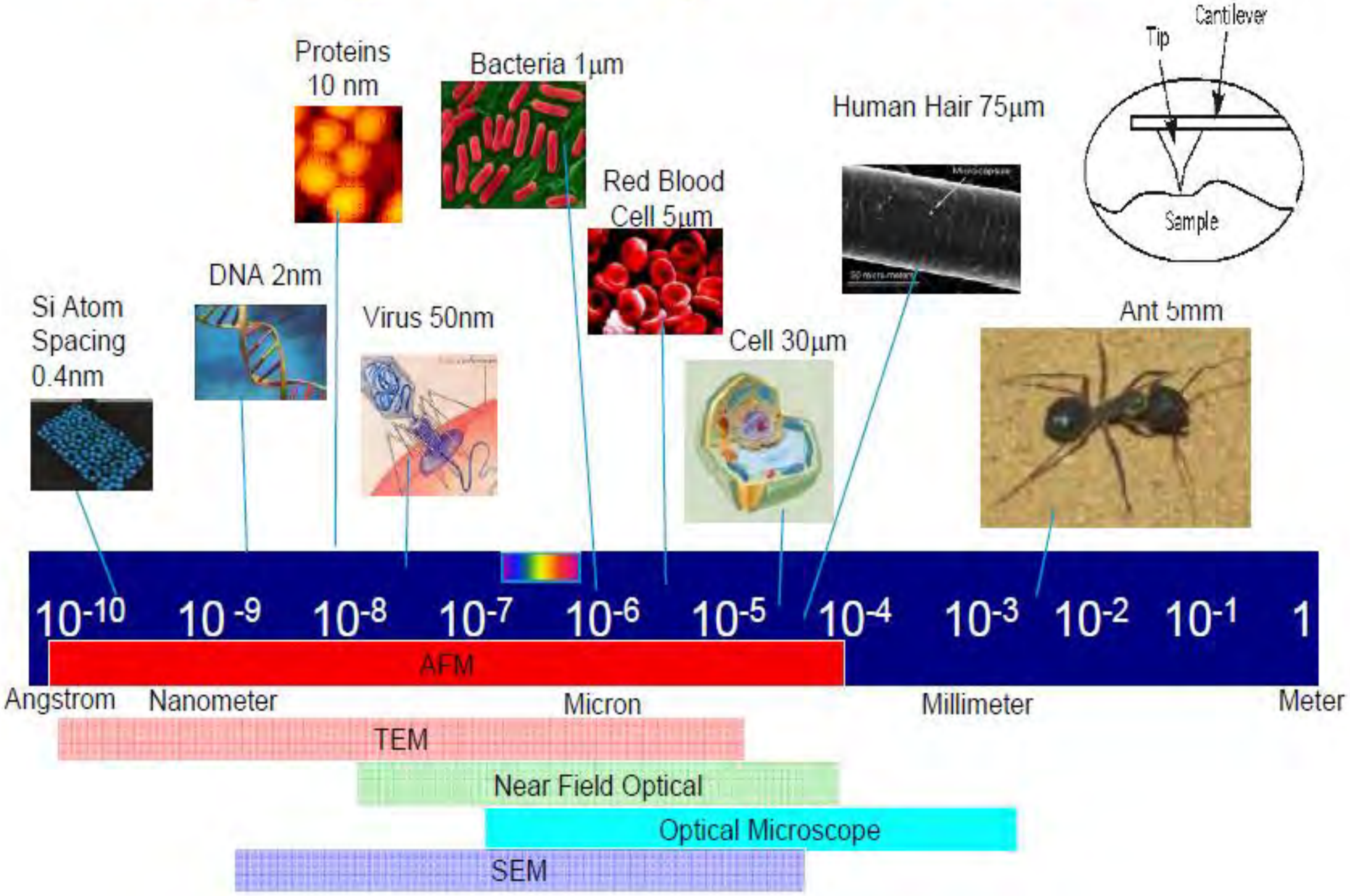
- **Optical Microscope**
  Suffers from diffraction effect on sample surfaces.
  Limited resolution at nanoscale.
- **Scanning electron microscope (SEM)**
  Require the use of electron beams at high vacuum environment and cannot be used for biological non-conductive samples and samples under liquid.
- **Atomic Force Microscopy (AFM)**
  Uses sharp probe scanning over the sample while maintaining a very close spacing to the surface . A tool to measure both topography and force-related material properties at the nanoscale.





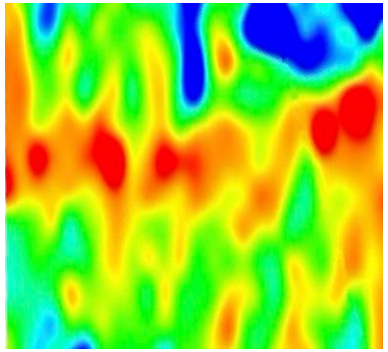


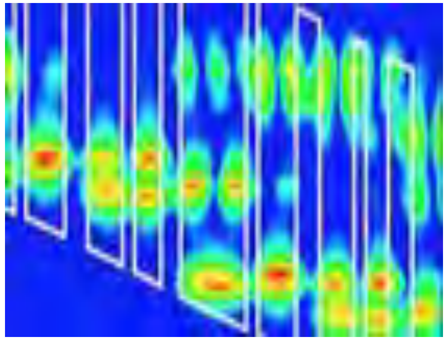
Imaging Techniques: Scales

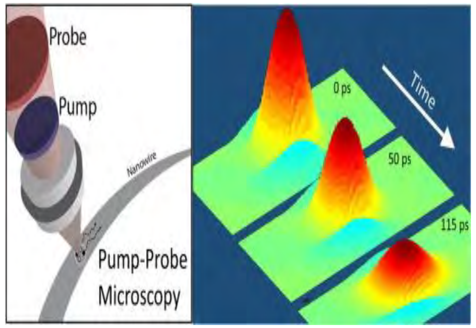


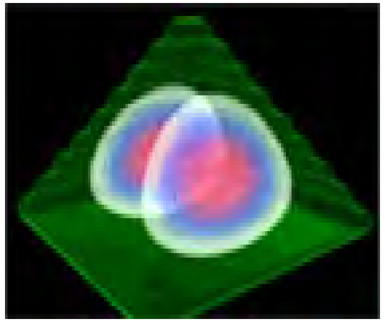
Visualization at the Nanoscale

Visualization of processes can be achieved by using laboratory instruments, online simulation and remote access instruments.









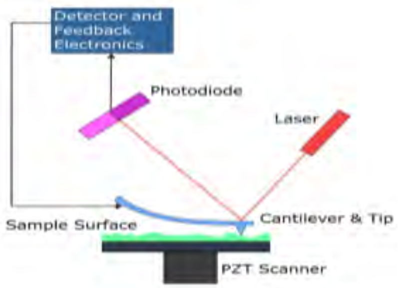
Learning through Visualization at the Nanoscale

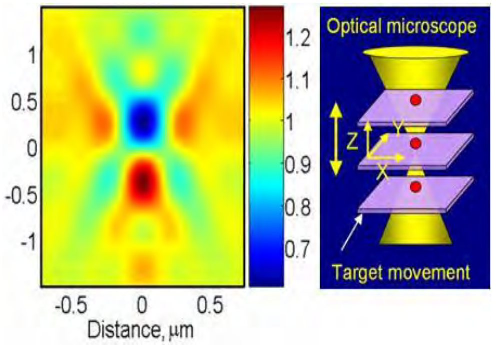
Types of Tools at RAIN

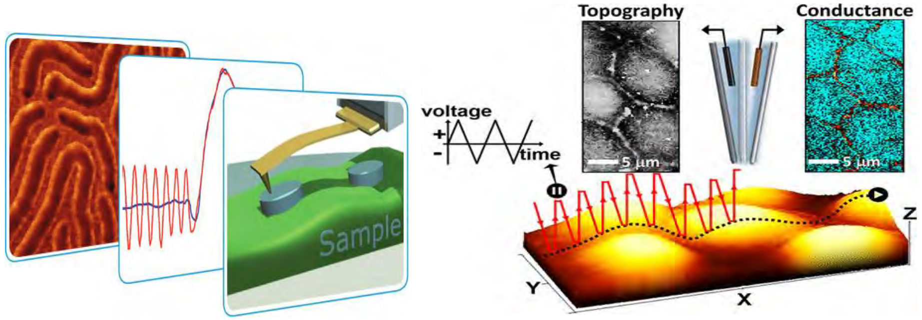
RAIN allows students to access and control microscopes and analytical tools, to look at nanosized materials from the ease of classrooms, or home computers, across the country.

Students control the tools over the Internet from 26 centers in real-time.

- Atomic Force Microscope (AFM)
- Optical Microscope
- Confocal Microscope
- Scanning Electron Microscope (SEM)
- Energy Dispersive Spectroscopy (EDS)
- Profilometer
- Ultraviolet–visible Spectrophotometer
- Molecular Analyzer
- Fourier Transform Infrared Spectroscopy (FTIR)
- X-ray fluorescence (XRF)
- Fabrication Tools





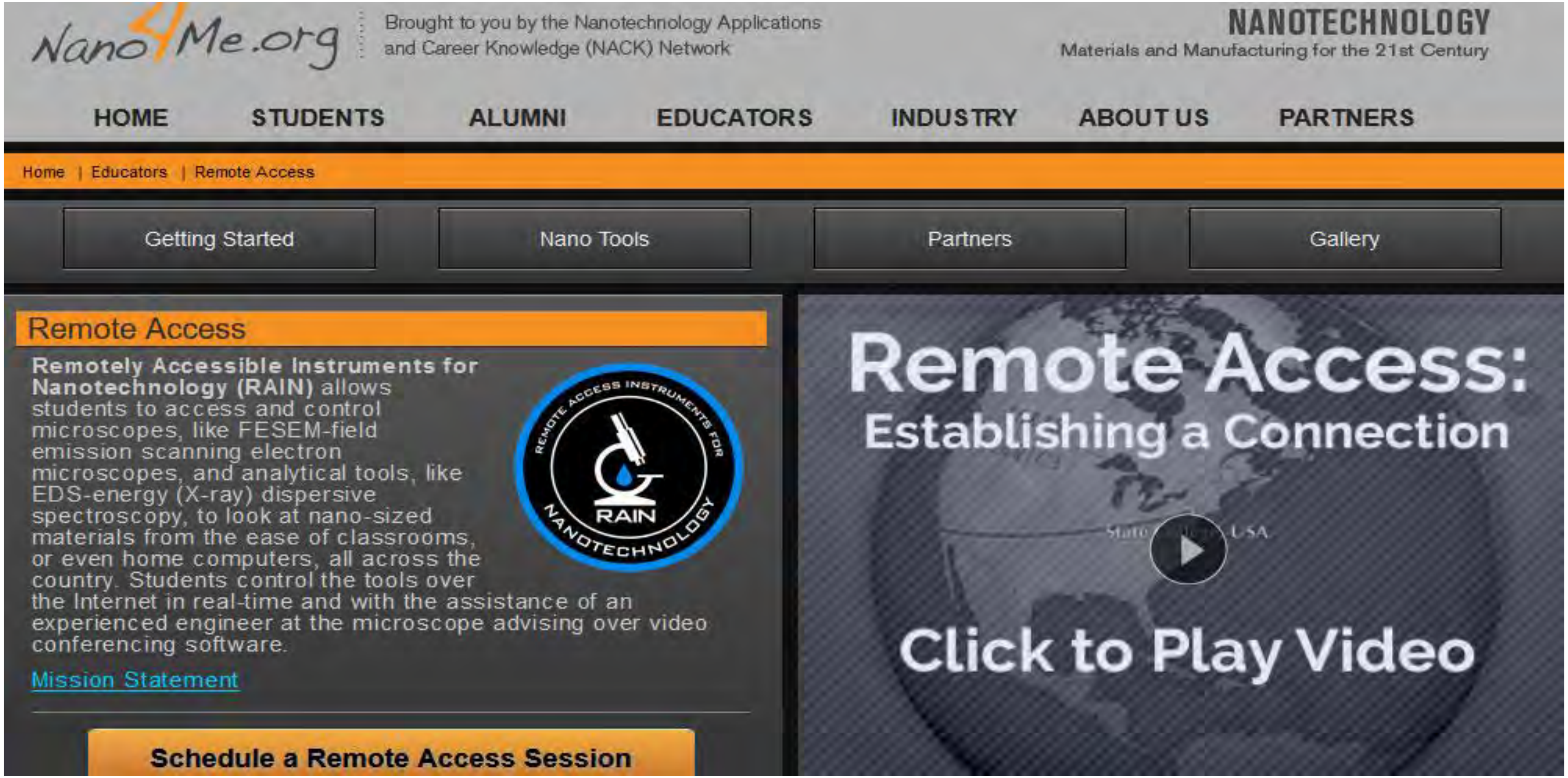


Online Tool/Methods For Visualizations

Remote Accessible Instruments for Nanotechnology (RAIN):
https://www.nano4me.org/remoteaccess

Benefits

- Saving on buying an expensive equipment
- Helps to train students before buying the equipment
- Introduces students to the processes and phenomenon at nanoscale


Nano4Me.org
Brought to you by the Nanotechnology Applications and Career Knowledge (NACK) Network
NANOTECHNOLOGY
Materials and Manufacturing for the 21st Century
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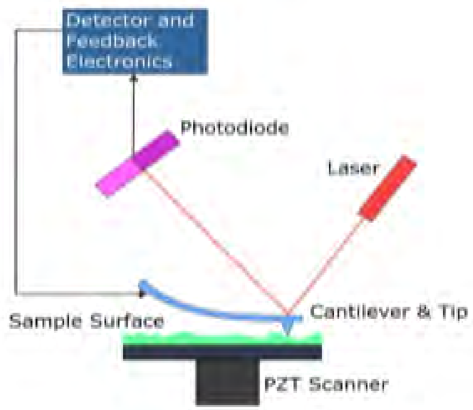
Nano Tools
Partners
Gallery
Remote Access
Remotely Accessible Instruments for Nanotechnology (RAIN) allows students to access and control microscopes, like FESEM-field emission scanning electron microscopes, and analytical tools, like EDS-energy (X-ray) dispersive spectroscopy, to look at nano-sized materials from the ease of classrooms, or even home computers, all across the country. Students control the tools over the Internet in real-time and with the assistance of an experienced engineer at the microscope advising over video conferencing software.
REMOTE ACCESS INSTRUMENTS FOR NANOTECHNOLOGY
RAIN
Mission Statement
Schedule a Remote Access Session
Remote Access:
Establishing a Connection
Click to Play Video

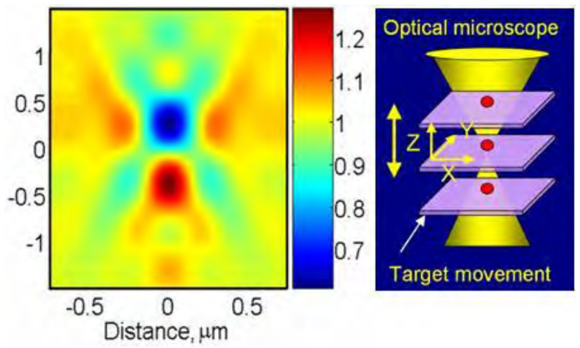

High Impact Technology Exchange Conference
HI-TEC
July 25–28, 2022
Grand America Hotel
Salt Lake City, UT

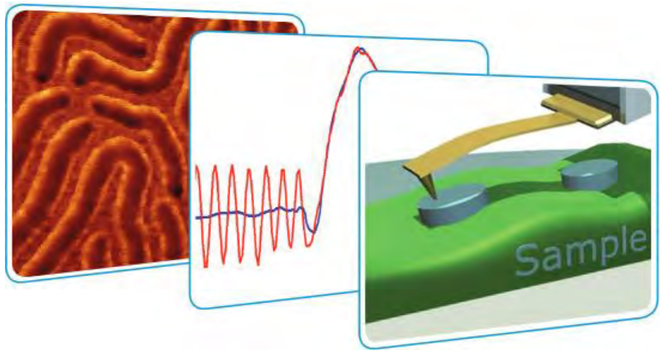
Learning through Visualization and Simulation at the Nanoscale
Remote Accessible Instruments for Nanotechnology (RAIN): Types of Tools

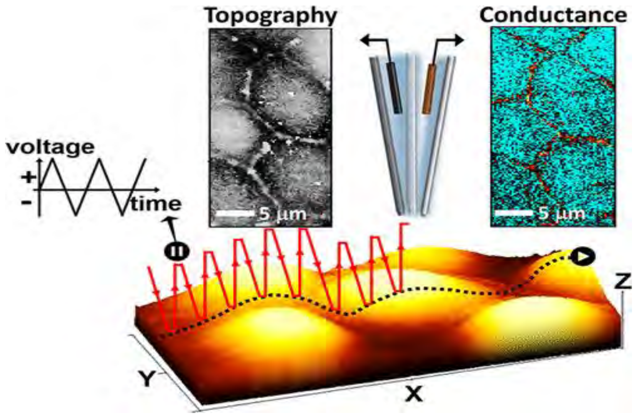
RAIN allows students to access and control microscopes and analytical tools, to look at nanosized materials from the ease of classrooms, or home computers, across the country. Students control the tools over the Internet from 26 centers in real-time.

- **Atomic Force Microscope (AFM)**
- **Optical Microscope**
- **Confocal Microscope**
- **Scanning Electron Microscope (SEM)**
- **Energy Dispersive Spectroscopy (EDS)**
- **Profilometer**
- **Ultraviolet–visible Spectrophotometer**
- **Molecular Analyzer**
- **Fourier Transform Infrared Spectroscopy (FTIR)**
- **X-ray fluorescence (XRF)**
- **Fabrication Tools**









RAIN Network Partner Locations

RAIN Network Intruments

nano4me.org/remoteaccess

RAIN Site	Remote Access Instruments
Arizona State University	SEM
Erie Community College	SEM/EDS
Forsythe Tech Community College	AFM
Northcentral Technical College	SEM, AFM, Flex AFM
North Seattle College	Confocal Microscope, AFM, Profilometer, SEM/EDS
Oakton Community College	SEM/EDS, Flex AFM, Profilometer
Pasadena City College	SEM/EDS
Pennsylvania State University	FESEM/EDS, SPM/AFM, Profilometer, UV-vis
Salt Lake Community College	SEM, AFM/SPM
University of Texas at San Antonio	SEM/EDS

Remote Accessibility of Nanotechnology Instruments

Atomic Force Microscope (AFM)

- Forsyth Tech Community College - (Nanosurf Flex Scan head AFM)
- Northcentral Technical College - (Nanosurf easyScan 2)
- North Seattle College - (Nanosurf easyScan 2)
- Oakton Community College - (Nanosurf easyScan 2 FlexAFM)
- Pennsylvania State University - (Bruker Innova)
- Salt Lake Community College - (Agilent 5400 AFM/SPM & Nanosurf easyS

Scanning Electron Microscope (SEM)

- NCI-SW at Arizona State University - (Phenom Pro)
- CABOCES - (Phenom ProX & JEOL-JSM-6010PLUS/LA)
- Erie Community College - (JEOL JSM-6010LA)
- Northcentral Technical College - (Hitachi TM 3030)
- Oakton Community College - (Hitachi TM 3000)
- North Seattle College - (Aspex EXplorer)
- Pasadena City College - (Phenom ProX)
- Pennsylvania State University - (ZEISS 55 Ultra FESEM)
- Research Triangle Nanotechnology Network - (FEI Quanta 200 Field Emission Gun)
- Salt Lake Community College - (Hitachi TM3000)
- SUNY Polytechnic Institute - (Hitachi TM3000 w/ x-ray (EDS))
- University of Texas at San Antonio - (Hitachi S5500 STEM)
- SCME at University of New Mexico - (Phenom ProX)

Optical Microscope

- Pennsylvania State University - (Leitz Ergolux)

A complete list is available at:
https://www.nano4me.org/remoteaccess#NanoTools

RETScreen Climate Database.

https://www.linkedin.com/pulse/retscreen-software-nasa-data-global-climate-solution-gregory-j-leng

The RETScreen Climate Database (i.e. long-term averages) includes the solar resource and meteorological data required in the feasibility analysis model. While running the software the user may obtain climate data from 6,700+ ground monitoring stations and/or from NASA's global satellite/analysis data. The ground-based stations for climate monitoring are situated in cities around the world and NASA global satellites are used to monitor populated regions in the remote areas where surface measurements are not available.

RETScreen is now used by more than 670,000 users in every country of the world, and in 36 languages that cover 2/3rds of the earth's population. In almost all projects that use RETScreen, the NASA data is used is some fashion, either to help assess the feasibility of a potential renewable energy, energy efficiency or cogeneration projects, or to measure and verify the ongoing energy performance of buildings, factories and power plants around the world.

How to Incorporate RAIN into your courses

Accessing RAIN Network

nano4me.org/remoteaccess

Step 1

Watch Videos: To get the most out of your remote access session, we suggest that teachers and students learn about the technology used to view things at the nano-scale level. Our recommended videos can be viewed in the classroom or assigned as homework.

Step 2

Complete the Remote Access Request Form: This is where you request a **remote test session** (if this is your first time running remote access with us) and a **live session**; select the **instruments** and **topic areas** you'd like to focus on; and provide your lab instructor with other important information such as your **class' interests** and **knowledge level**.

Step 3

Run a remote test session

º This is used to check your audio, video, and Internet connections.

º Takes about 20 minutes.

Step 1

Before you start remote access, you'll need to:

1. Install Video Conferencing Software

Based on the instrument and partner site you requested, you will need either Zoom or Team Viewer. Both are free to download and use.

2. Set up your computer. You need:

º Webcam
º Microphone
º Speakers
º A projector or large display is recommended, but not require

Step 3

Choose your samples: You can use in house samples or send your own to the remote access site you selected when scheduling your session. Based on your remote access request (step 2), a remote access manager will reach out to you regarding in house sample availability and to provide address information for any samples you wish to mail in.

Step 4

Run a live session

º This is where you will have live remote access to the lab equipment.
º This can take anywhere from 15 minutes to 2 hours.

Step 5

Give us feedback!

Help us show the NSF that remote access is a valuable resource.

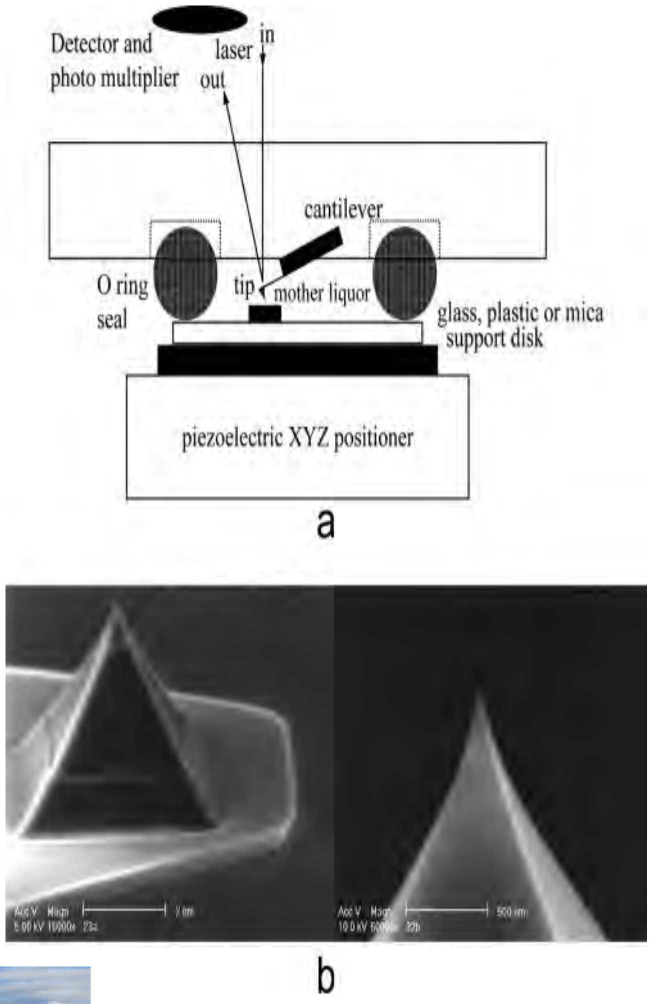
How to Incorporate RAIN into your courses

Accessing RAIN Network

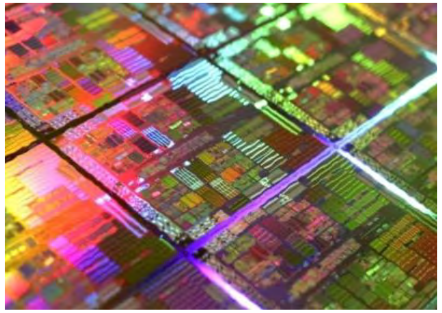
nano4me.org/remote access

Advantages of AFM Visualization for Biological Structures

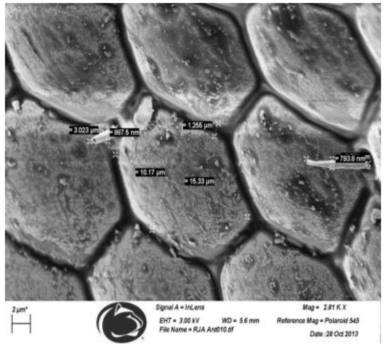
- Visualize the structure of viruses at high resolution ranging from a nanometer to hundred microns
- Non-destructive and non-intrusive
- Visualization of virus samples can be carried on the surface of cells in situ, in fluids and air, or post histological procedures
- Does not disturb the specimen from its natural state
- Can be used to identify and study membranes, RNA and DNA, and protein assemblies and their structures
- Relatively inexpensive and portable
- Requires minimal quantity of samples for measurements
- Can be linked with other molecular techniques such as EM or PCR (*Polymerase chain reaction)*



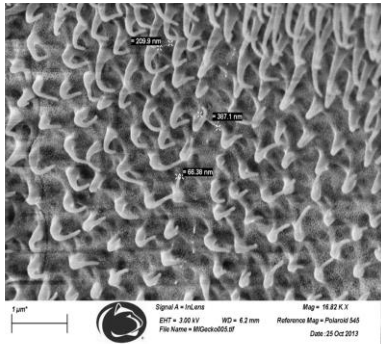
Nanoscale images are captured with the same tools available for the users at RAIN.



Microchip



Gecko



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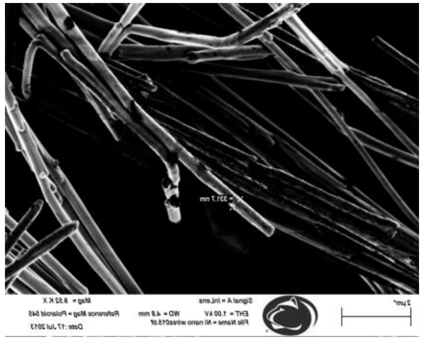
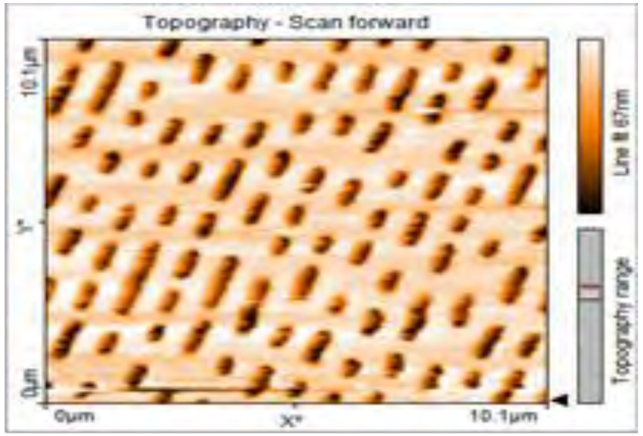


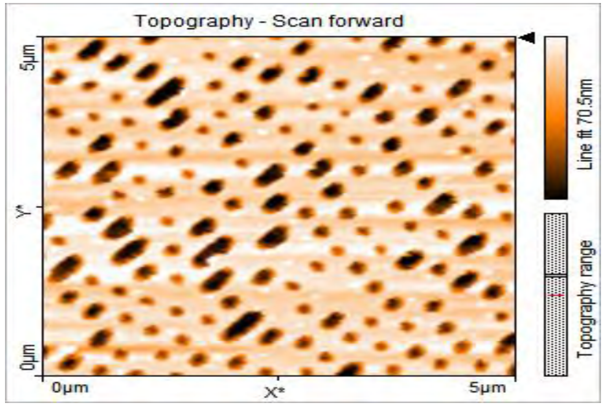
Ni nanowire

Visualization of digital video discs (DVDs), and BluJay DVDs

Objective: To study the nanoscale features and determine density of information by direct measurement of the patterns and tracks using NanoSurf EasyScan 2 AFM in the Intermittent contact (tapping mode) .

Video data requires significantly more storage density and in order to accommodate the data, the pit and land sizes must be shrunk to smaller values. The spacing between tracks, width of tracks, their depth and reflectance vary according to the type of disc. Measuring the physical characteristics of the disc can help calculate the storage capacity of the disc. The smallest features of the DVDs are pits about 400 nm long, 320 nm wide, 120 nm deep, with a track pitch of 740 nm. BluRay DVD players provide high definition video for HDTV, requiring more data density. On Blu-ray the pits are written on about 300 nanometer wide tracks, which is less than half the width of a DVD as shown in the following figures.





Detection of Viruses using Nanoscale Visualization

Most single virus particles measure about 20 to 250 nm in diameter with some measuring up to 1000 nm. Key techniques widely used for the visualizations are:

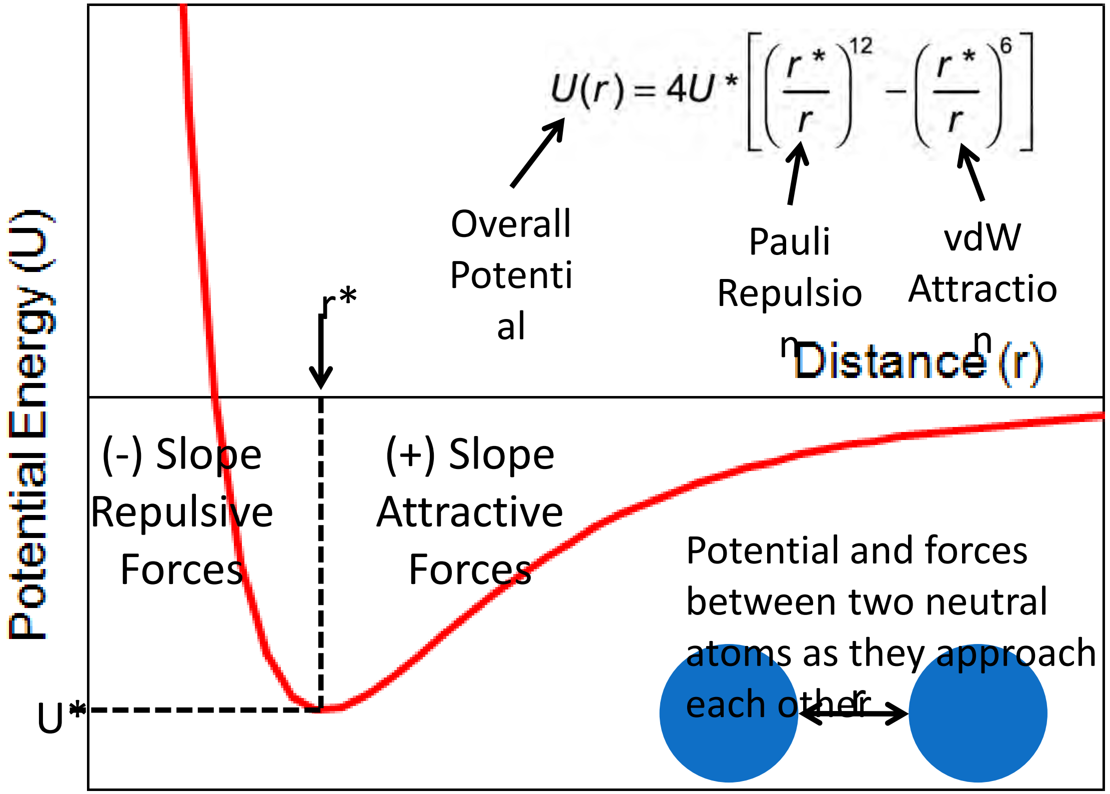
- **Electron Microscopy**
- **X-Ray Diffraction Analysis**

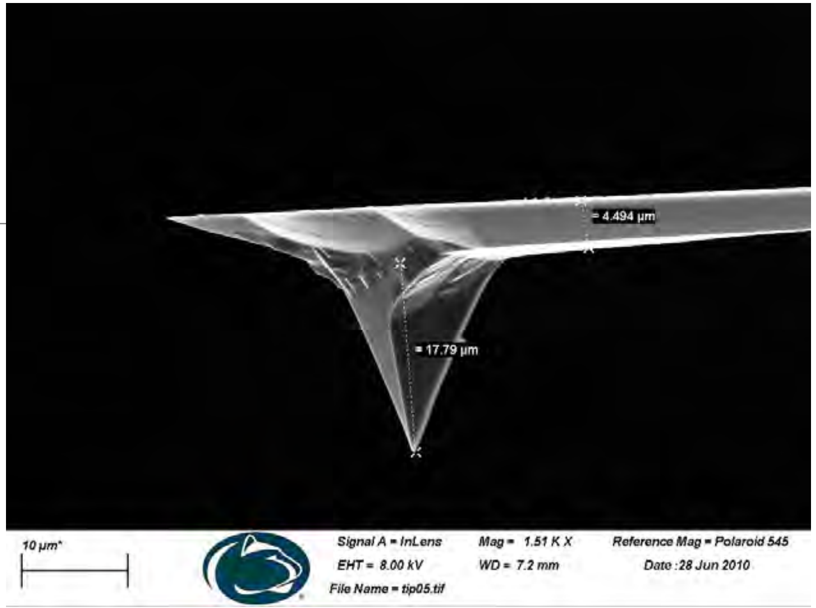
These techniques require expensive equipment, difficult to install and cannot be used for live biological samples as compared to Atomic Force Microscopes which is inexpensive, easy to install, smaller in size with additional features.

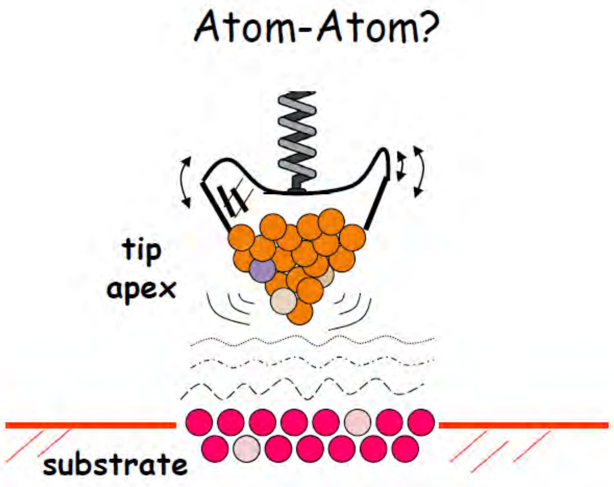
Avian influenza Virus Common cold Infection, dentate bacterial virus PNG

AFM Overview

Intermolecular Forces

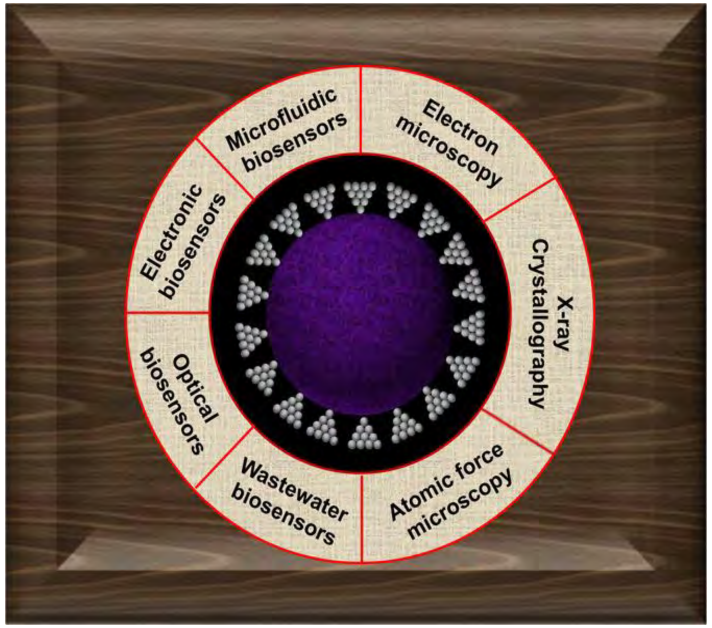






Application of Atomic Force Microscopy (AFM) in Imaging of Viruses and Virus-Infected Cells*

- AFM is nonintrusive and nondestructive; can be applied to soft biological samples, particularly in cases when tapping mode is employed.
- Samples can be imaged in air or in fluids (including culture medium or buffer), in situ on cell surfaces, or after histological procedures.
- In principle, only a single cell or virion need be imaged to learn of its structure, though normally images of as many as is practical are collected.
- AFM produces 3D, topological images that accurately illustrate the surface traits of the virus or cell under study.
- The AFM images are like common light photographic images.
- The structural shapes of viruses observed by AFM are in harmony with models derived by X-ray crystallography and cryo-EM.



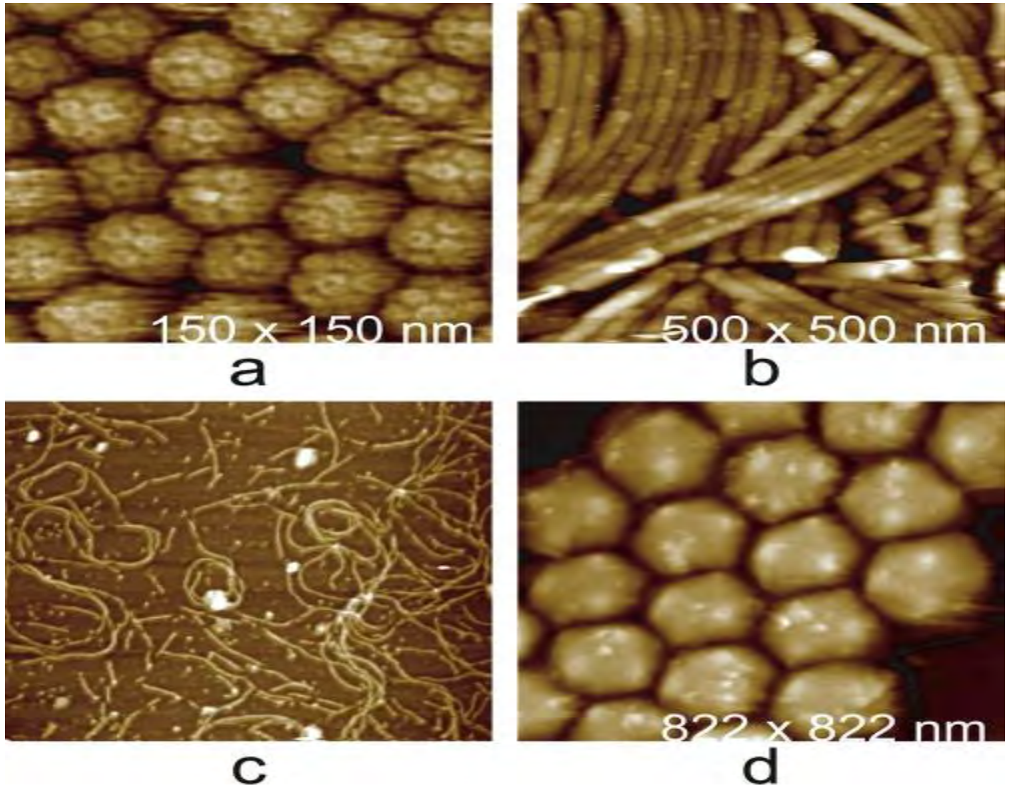
Opportunities and Challenges for Biosensors and Nanoscale Analytical Tools for Pandemics: COVID-19*

*https://www.ncbi.nlm.nih.gov/pmc/articles/PMC7319134/

* Yurii G. Kuznetsov and Alexander McPherson
https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3122623

Example of the Application of Atomic Force Microscopy in Imaging of Viruses and Virus-Infected Cells*

AFM images. (a) Condensed mass of brome mosaic virus (BMV), a T = 3 icosahedral virus that infects grasses such as barley. (b) Helical, rod-shaped tobacco mosaic virus (TMV), a ubiquitous pathogen throughout the plant world. (c) Tangles of marine filamentous bacteriophage and their broken fragments scattered on the AFM substrate. (d) Virions of Tipula iridescent virus, a very large icosahedral virus that infects insects. The virions of BMV have a diameter of 30 nm, TMV is about 20 nm in diameter and1,000 nm in length, and the adenovirus and iridovirus have diameters of about 100 nm and 200 nm, respectively.



***Atomic Force Microscopy in Imaging of Viruses and Virus-Infected Cells**

Yurii G. Kuznetsov and Alexander McPherson*

https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3122623/

MODELING AND SIMULATION OF PV SYSTEMS AND SOFTWARE TOOLS

To understand the capabilities, limitations, and potential of current and future PV systems can be achieved by using modeling and simulation software to design, analyze and estimate not only the PV systems but also the cost of production of energy. Modeling and simulation tools can be classified into:

- Prefeasibility study
- Design
- Analysis
- Sizing
- Dynamic behavior of the system.

It is desirable that simulation software should address consideration of simulation and modeling capabilities, hardware and software issues, and consideration of input and output. Many software tools both from private industry and government agencies have been developed and the availability is becoming common as the cost is reduced and

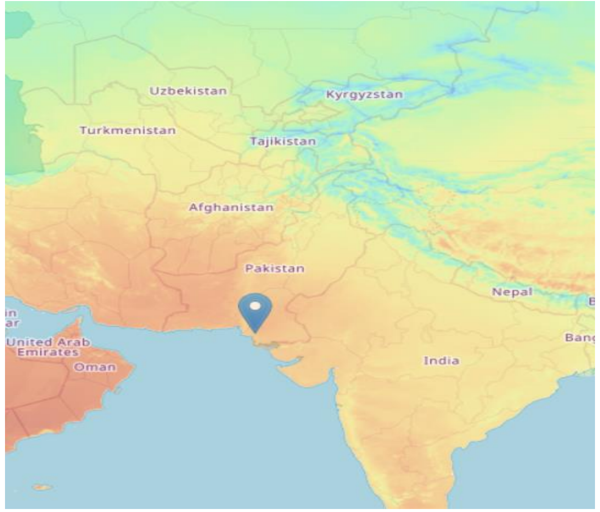
Online Web Based Software

PV resources https://www.pvresources.com/en/software/software.php has listed over 50 photovoltaic software tools in the following categories.

● Economic evaluation tools
● Photovoltaic industry related tools
● Analysis planning tools
● Smart phone apps
● Monitoring and control tools
● Site management tools
● Site analysis tools● Solar radiation maps and data● Online tool

Photovoltaic Geographical Information System (PVGIS)

http://re.jrc.ec.europa.eu/pvgis/apps4/pvest.php



PVGIS provides free and open access to:

- PV potential for different technologies and configurations of grid connected and stand-alone systems.
- Solar radiation and temperature, as monthly averages or daily profiles.
- Full time series of hourly values of both solar radiation and PV performance.
- Typical Meteorological Year data for nine climatic variables.
- Maps, by country or region, of solar resource and PV potential ready to print.
- PVMAPS software includes all the estimation models used in PVGIS.

PVGIS is available in English, French, Italian and Spanish for any location in Europe and Africa, as well as large part of Asia and America.

It was developed by the joint Research Center in Italy and funded by European Commission

SolarGIS

(http://solargis.info)

It is online tool which allows access to high-resolution solar data, other meteo data, PV simulation software, solar maps, GIS database, PV monitoring services for solar energy. It incorporate PV planner https://solargis.info/pvplanner/#tl=Google:roadmap&bm=map&loc=-30.25803,118.806325

A new generation web service) aimed to increase efficiency and reduce uncertainty in planning and performance assessment of PV systems. SolarGIS is based on more than 10 years of R&D, international collaboration, and experience with previous projects, such as PVGIS.

FIGURE C.9 Monthly electric potential of Geraldton, Australia.

PVsyst (http://www.pvsyst.com/en)

PVsyst is designed to be used by architects, engineers, and researchers. It is also a very useful educative tool. PVsyst is able to import meteo data, as well as personal data from many different sources.

New features which are available in PVsyst 7:

- **Support of 64-bit architectures** : extension of PVsyst capabilities of handling large projects and shading scenes
- **Irradiance:** new improved treatment of the circumsolar component, impacts on the electrical shadings and vertical Bi-facial systems
- **System :** unlimited number of sub-arrays
- **Shadings :** conversion of fixed tables to trackers, new trackers with central gap parameter for bifacial
- **Output AC circuit :** definition of several MV and HV transformers, with their specifications
- **Live results display** : see results values and graphs while the simulation is running
- **Economic evaluation** : Levelized Cost of Energy (LCOE), Net Present Value (NPV), multiple loans of multiple types, advanced depreciation configuration
- **Economic evaluation** : availability for Stand-alone and Pumping systems
- **Simulation :** display of warnings during the simulation and with the results
- **Module Layout :** great improvements in submodule shading calculations accuracy, print of the layout has also been improved and can now be printed in the report
- **User interface :** improvements of the user interface and user experience
- **Localization :** full-software translation coverage (except the Help), Turkish and Korean languages available

NREL's PVWatts® Calculator https://pvwatts.nrel.gov/

Estimates the energy production and cost of energy of grid-connected photovoltaic (PV) energy systems throughout the world. It allows homeowners, small building owners, installers and manufacturers to easily develop estimates of the performance of potential PV installations.

NREL's PVWatts® is a web application developed by the National Renewable Energy Laboratory (NREL) that estimates the electricity production of a grid-connected roof- or ground-mounted photovoltaic system based on a few simple inputs.. PVWatts® is suitable for very preliminary studies of a photovoltaic system that uses modules (panels) with crystalline silicon or thin film photovoltaic cells.

To get started with PVWatts®, type the street address, zip code, or latitude and longitude of the system's location, and click **GO**. PVWatts® uses this information to automatically identify solar resource data available at or near the system's location. To represent the system's physical characteristics, PVWatts® requires values for six inputs:

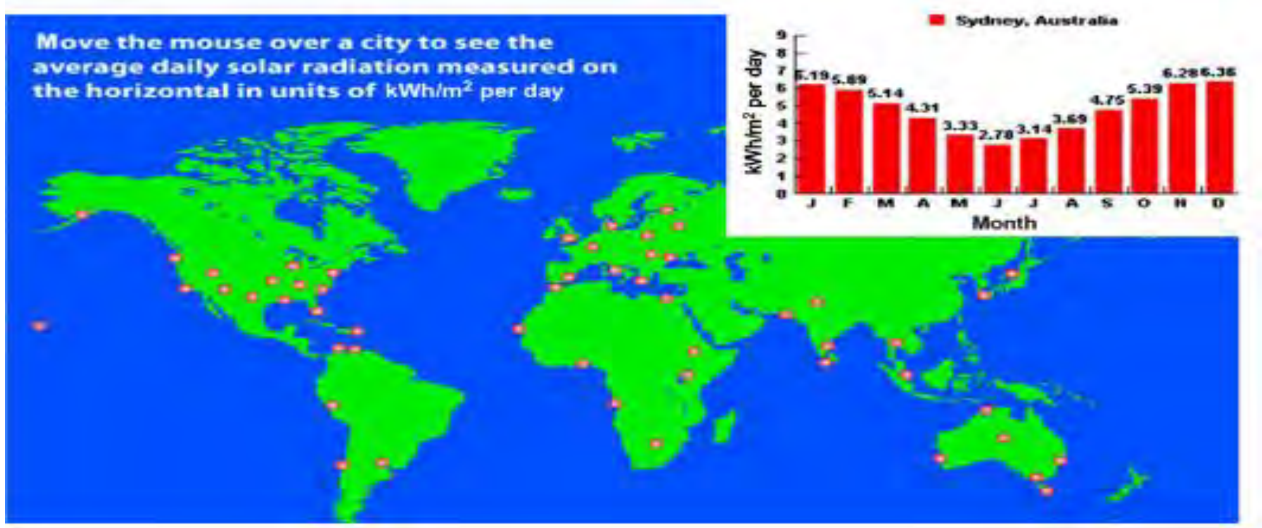
- DC system size
- Module type
- Array type
- System losses
- Array tilt angle

NREL is a national laboratory of the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, Operated by the Alliance for Sustainable Energy, LLC. PVWatts® is a registered trademark by Alliance for Sustainable Energy, LLC in Golden, CO, 80401. Version 6.2.4

Solar Insolation for Global Locations Using the Photovoltaic Education Network

http://www.pveducation.org/pvcdrom/properties-of-sunlight/average-solar-radiation#

A quick way of estimating and comparing solar insolation for global locations can be obtained by accessing this website with about 50 marked localities. These locations represent metropolitan areas in different part of the world including Asia, Africa, Australia, Europe, North and South America. In order to find solar insolation, one has to point the cursor to one of the locations on the world map. The result will be a bar graph showing the average daily radiation measured on the horizontal in units of kWh/m2 per day for each month of the year. This online tool was developed by Christiana Honsberg and Stuart Bowden of Arizona State University, USA, and is part of an electronic textbook (available at http://www.pveducation.org) and on CDs. The material contained in the electronic book is based in part upon work supported by the National Science Foundation grant.



Online Databases for Solar Radiation

There are more than 20 solar radiation databases which can be accessed online at http://www.photovoltaic-software.com/solar-radiation-database.php.These databases can be used to estimate solar radiation or solar insolation for locations in the United States and the world. Given below are some of the databases.

SOLARGIS FORECAST

•SOLARGIS FORECAST offers a real-time satellite-based forecasting and nowcasts based on Solargis models.

- High-quality nowcasting up to next 6 hours and forecasts up to 10 days
- Available for any site globally
- PV power

•Solcast - Solar Irradiance Data

•Solcast - Solar Irradiance Data Solcast offers global coverage of historical (up to 15y), recent (past 3 months) and live (past 7 days) solar irradiance data. Free data access for researchers and hobbyists (home PV system use)....

•How to get solar radiation and climate data (precipitaton, temperature, wind, insolation...) anywhere in the world free from NASA database?

•**Get worlwide climate data for free from NASA in 3 steps ?**

This tutorial helps you to get free set of meteorological data from NASA database through the POWER DATA ACCESS VIEWER online free tool.

•Global Solar Atlas - PV Power simulation

•Global solar Atlas provides a summary of solar power potential and solar resources globally. It also provides an online free PV power simulation tool.

•Global Solar Atlas

•Global solar Atlas provides a summary of solar power potential and solar resources globally. It is provided by the World Bank Group ...

•NASA SSE

•NASA SSE NASA Solar Radiation Archive of over 200 satellite-derived meteorology and solar energy parameters, globally available at a resolution of 1x1 degrees. New! See our tutorial to get monthly and annual worldwide solar and climate data...

RETScreen Climate Database

https://www.linkedin.com/pulse/retscreen-software-nasa-data-global-climate-solution-gregory-j-leng

The RETScreen Climate Database (i.e. long-term averages) includes the solar resource and meteorological data required in the feasibility analysis model. While running the software the user may obtain climate data from 6,700+ ground monitoring stations and/or from NASA's global satellite/analysis data. The ground-based stations for climate monitoring are situated in cities around the world and NASA global satellites are used to monitor populated regions in the remote areas where surface measurements are not available.

RETScreen is now used by more than 670,000 users in every country of the world, and in 36 languages that cover 2/3rds of the earth's population. In almost all projects that use RETScreen, the NASA data is used is some fashion, either to help assess the feasibility of a potential renewable energy, energy efficiency or cogeneration projects, or to measure and verify the ongoing energy performance of buildings, factories and power plants around the world.

Best Practices
and
Sample Experiments for Lecture Support
at PSU & GVSU

Order of Presentation

- Fusion of 4the Industrial Revolution (4IR)Technologies: Challenges and Opportunities for Academia
- Online Tools for Visualization and Simulations
  - NanoHub
    - Examples of simulations using nanoHub
  - Phet Interactive Simulations
  - Physicell
  - CompuCell3D
    - Examples of Simulation of Covid-19 Virus
  - RAIN: Remote Accessible Instruments for Nanotechnology
    - AFM Application for visualization of Viruses
  - PV Systems modeling and simulation tools
- Best Practices and Sample Experiments to Support Lectures at PSU & GVSU
    - Examples of XPS & XRD
- Student Reception and Applicability
- First Time use tips for Instructors
- Conclusion
- Q & A

Incorporating X-ray Characterization with Simulation Tools in Lectures at PSU & GVSU

XPS and XRD

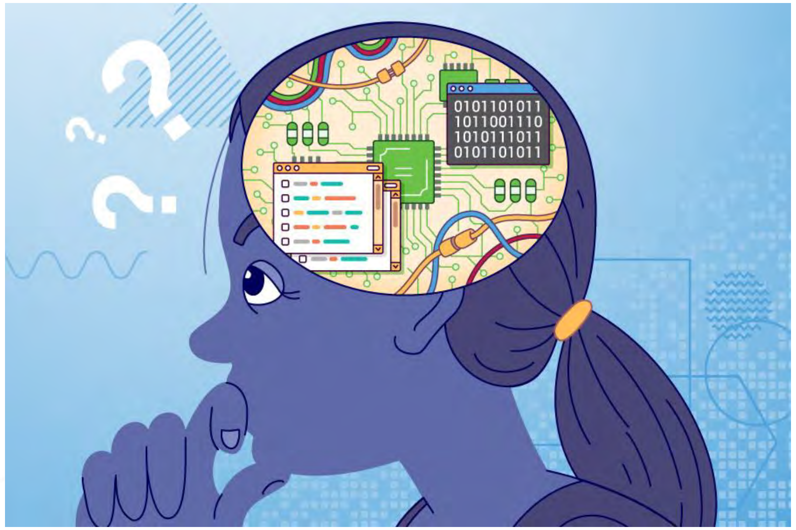
Grand Valley State University
Seymour and Esther Padnos College of Engineering and Computing

Atilla Ozgur Cakmak
Assistant Professor
Electrical Engineering
Grand Valley State University

Simulation-full classrooms

Covid19 C.E. Teaching

https://newlearningonline.com/learning-by-design/pedagogy



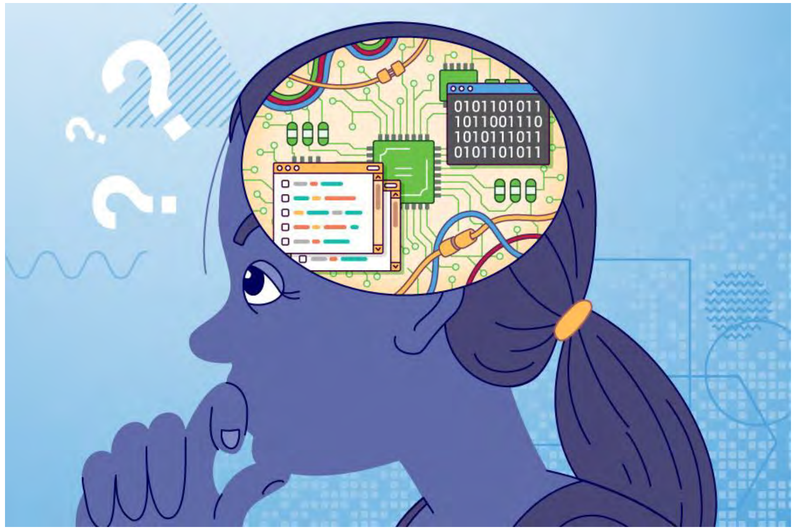
https://teachcomputing.org/pedagogy

https://www.isglobal.org/healthisglobal/-/custom-blog-portlet/how-covid-19-has-changed-the-way-we-teach-and-learn-in-our-master-s-programmes/6114383/0

https://www.nature.com/articles/d41586-020-00896-7

Simulation-full classrooms

https://newlearningonline.com/learning-by-design/pedagogy



https://teachcomputing.org/pedagogy

https://www.freepik.com/free-vector/cartoon-empty-laboratory-room_13248590.htm

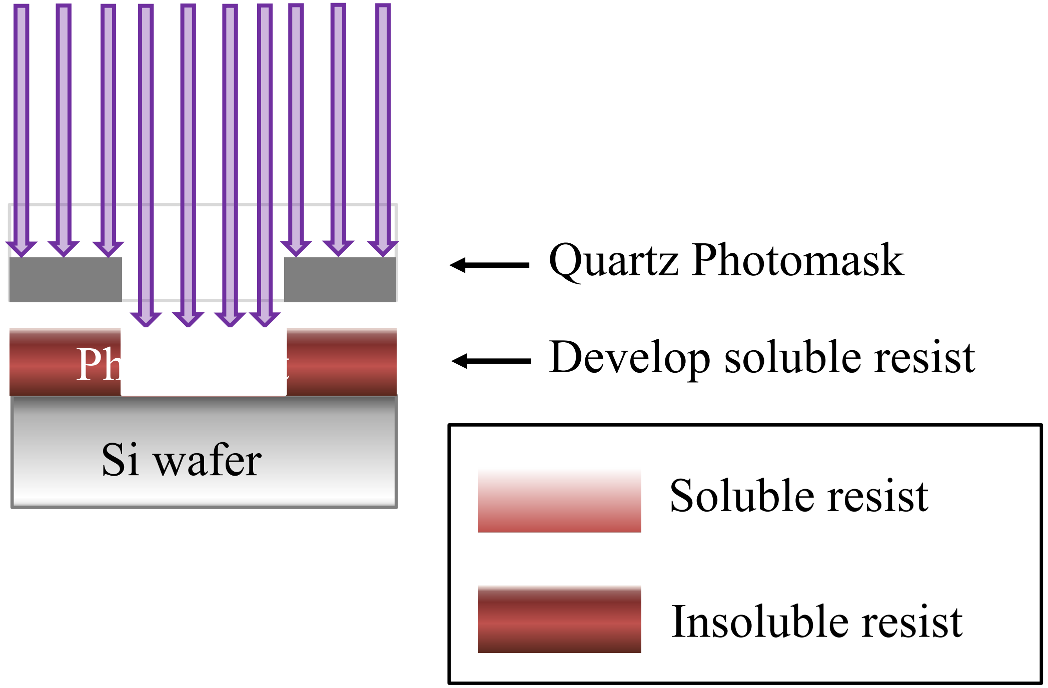

High Impact Technology Exchange Conference
HI-TEC
July 25–28, 2022
Grand America Hotel
Salt Lake City, UT

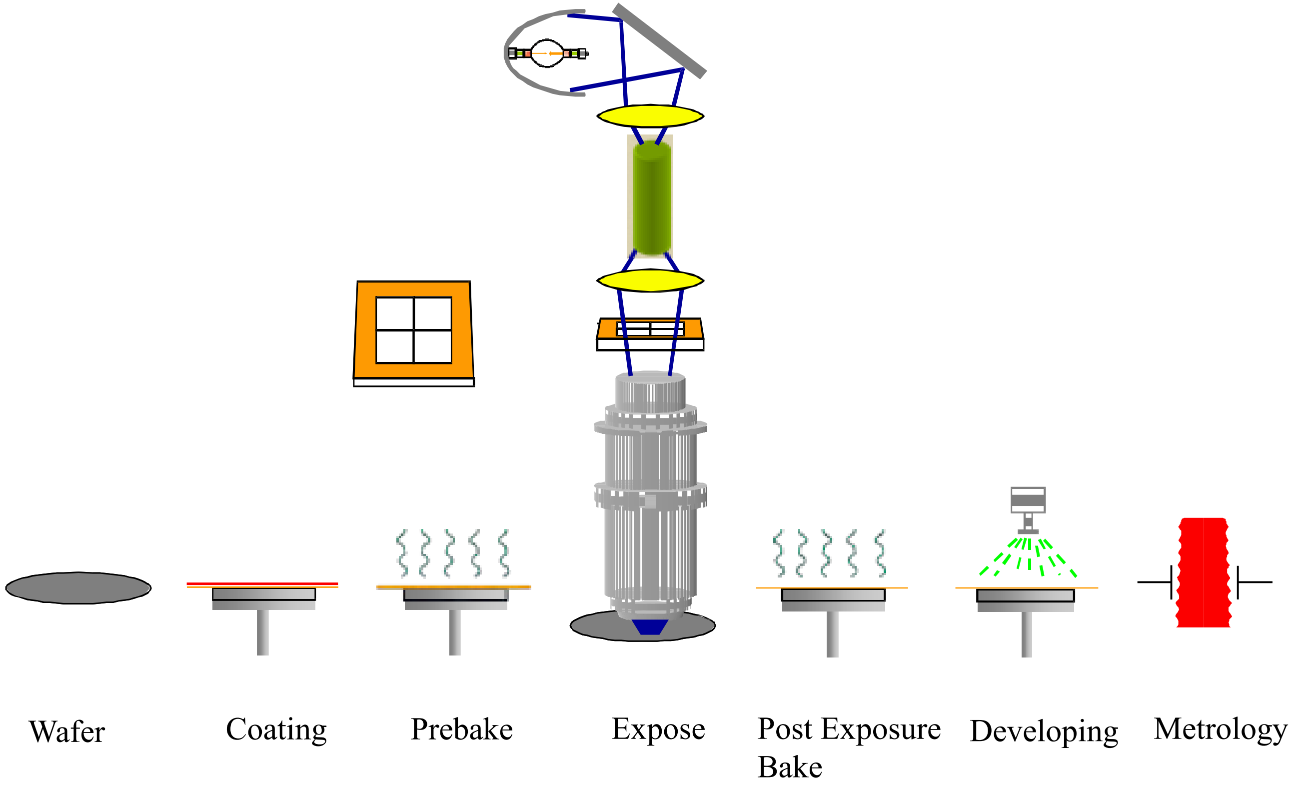

You sure they're absorbing all of this?
TRAINING & COMMUNICATIONS


HI, COME ON IN.
THANKS, PROF. SMITH.
READY?
rdfgh.
FWWOOSH!
JORGE CHAM © 2007
WWW.PHDCOMICS.COM

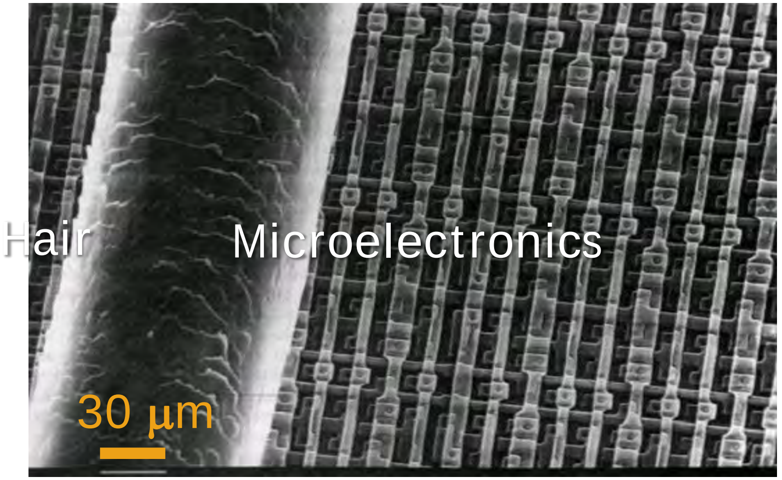
A lithography training tool

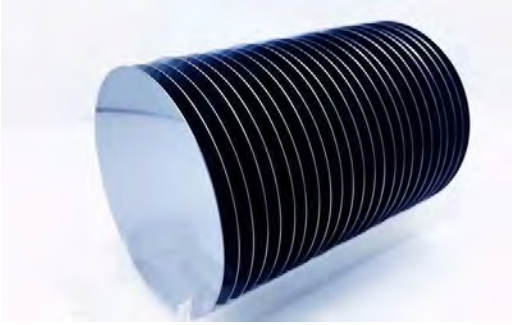
This was an example of positive lithography: What shows goes

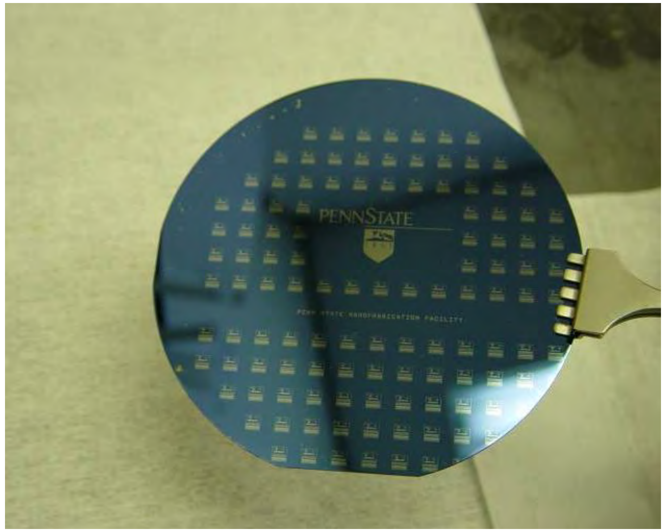




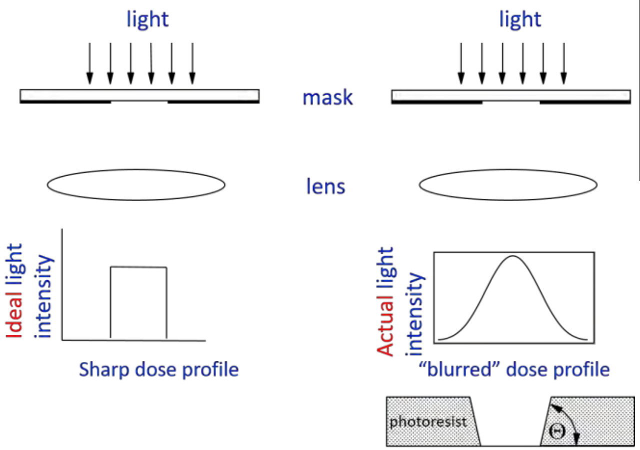
A lithography training tool



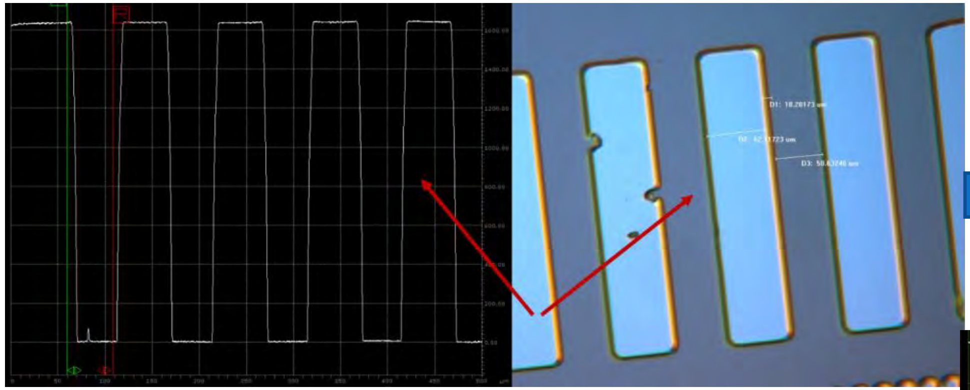




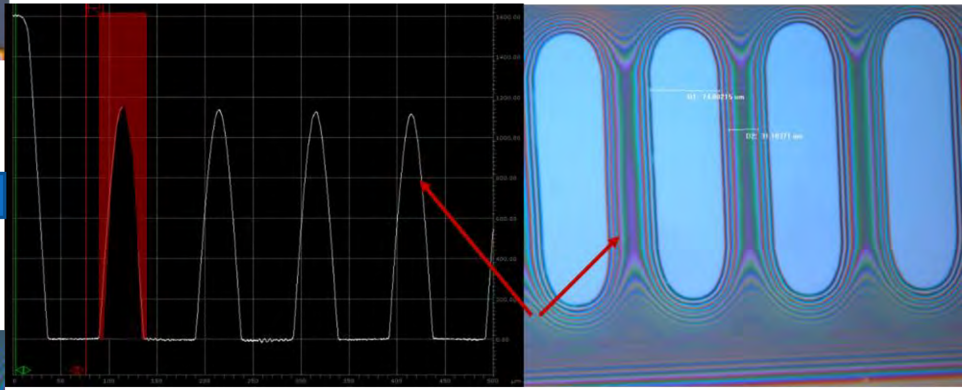
A lithography training tool



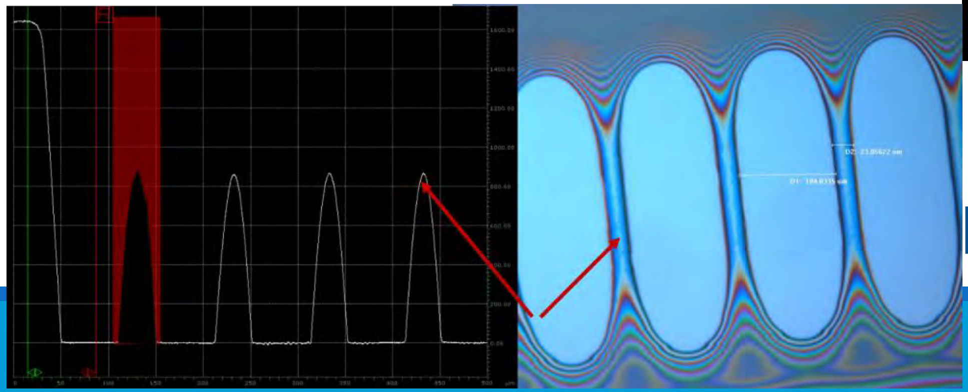
Positive Photoresist (Shipley 1813) results
Profilometer Scan (left) – Optical Microscope (right)



Ideal Exposure: 26 seconds



Over Exposure: 30 seconds



Over Exposure: 36 seconds

A lithography training tool

More about it here: https://sid.onlinelibrary.wiley.com/doi/full/10.1002/jsid.1067

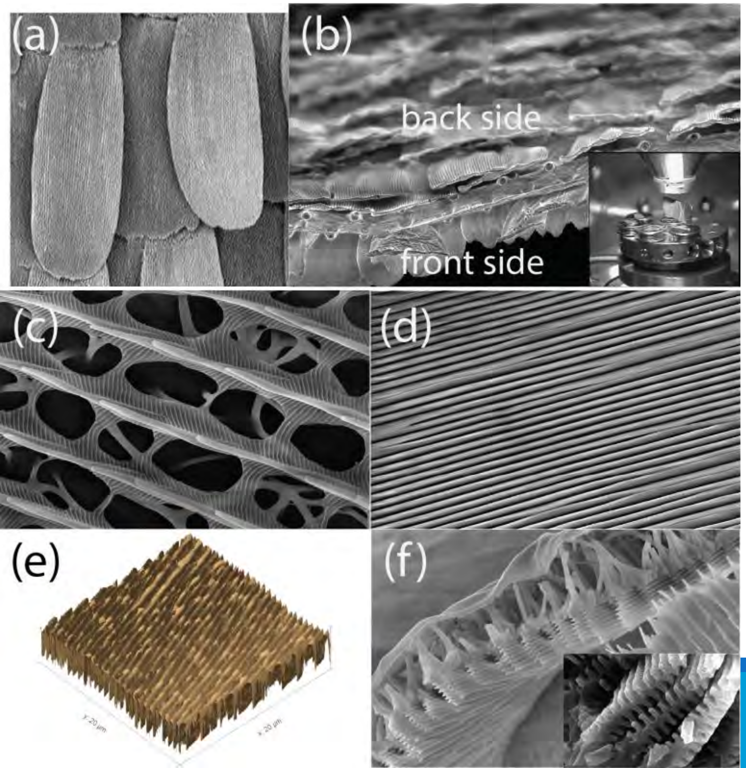
Under the observations, comment on the famous formula of $\boldsymbol{R = k_1 \frac{\lambda}{NA}}$ in the world of lithography.

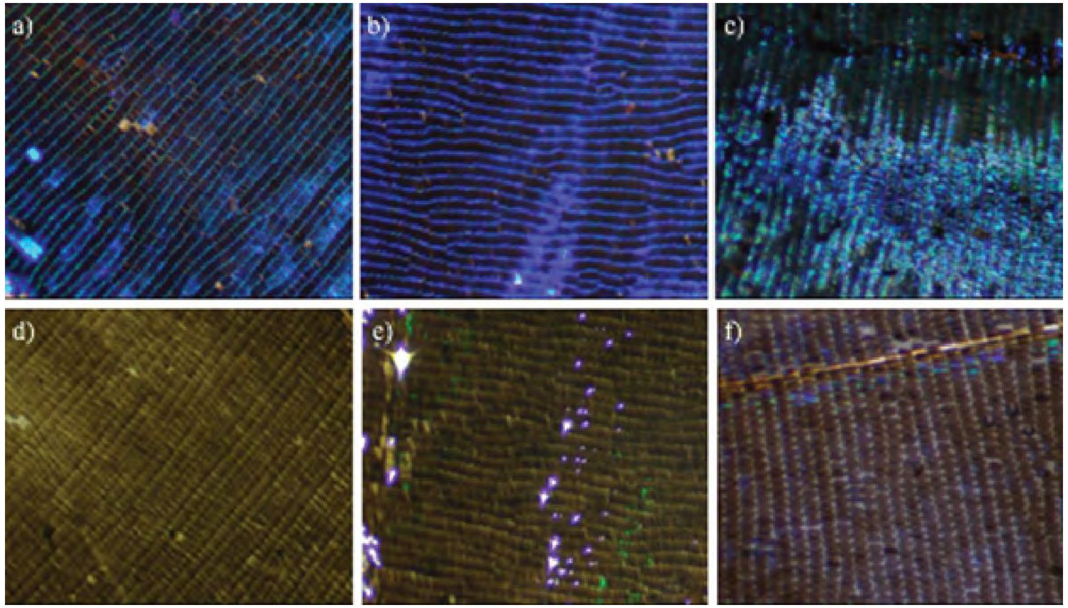
TABLE 1 Summary of the activities in Scenario 1 with the given parameter settings

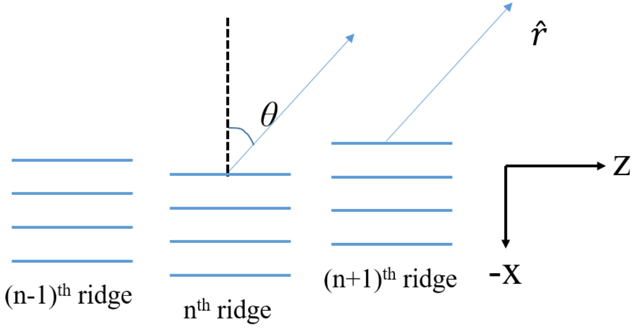
Period (nm)	λ (nm)	NA	Exposure time (s)	Comments
600	193	0.5	2	Severe underexposure/underdevelopment
600	193	0.5	22.5	Ideal exposure time to obtain 300-nm spaces
300	193	0.5	22.5	Could not resolve (below limit)
300	193	0.96	22.5	Resolved: 146-nm-wide spaces
300	13	0.5	22.5	Resolved: 149-nm-wide spaces Notice the sharp slopes

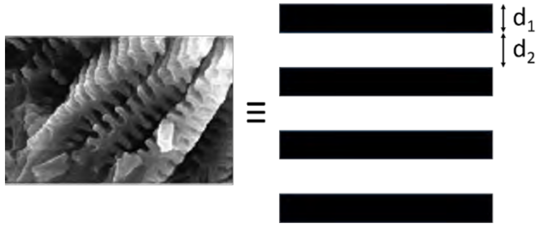
Note: The rest of the parameters have default settings; students can hit "Set0" button to retrieve them.

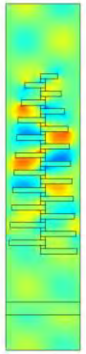
Thinking a butterfly wing as an antenna array



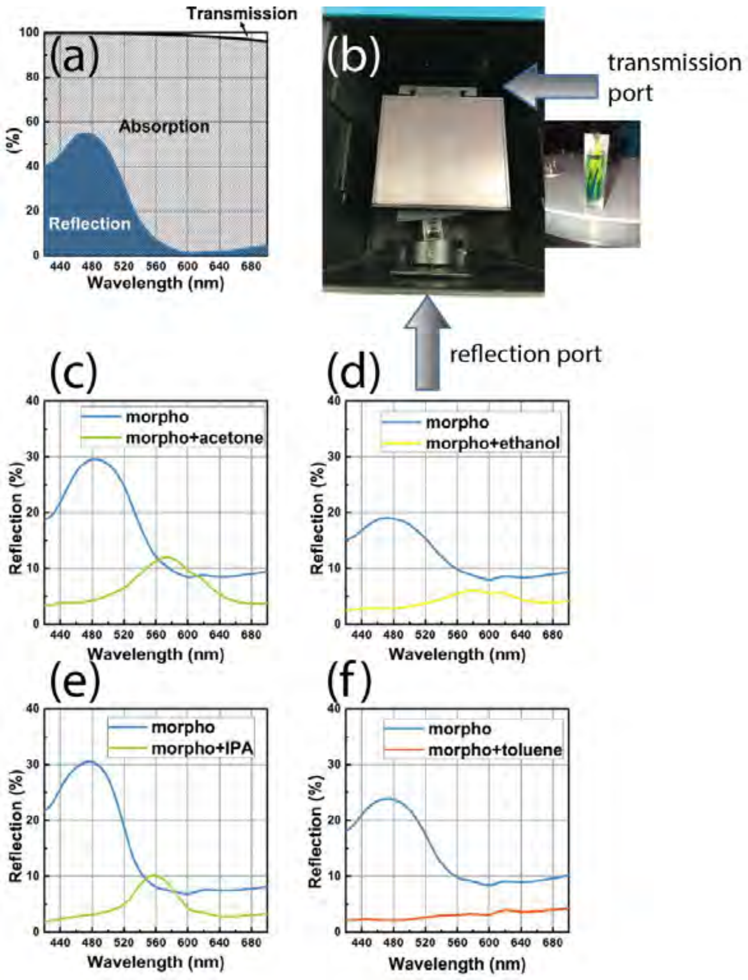


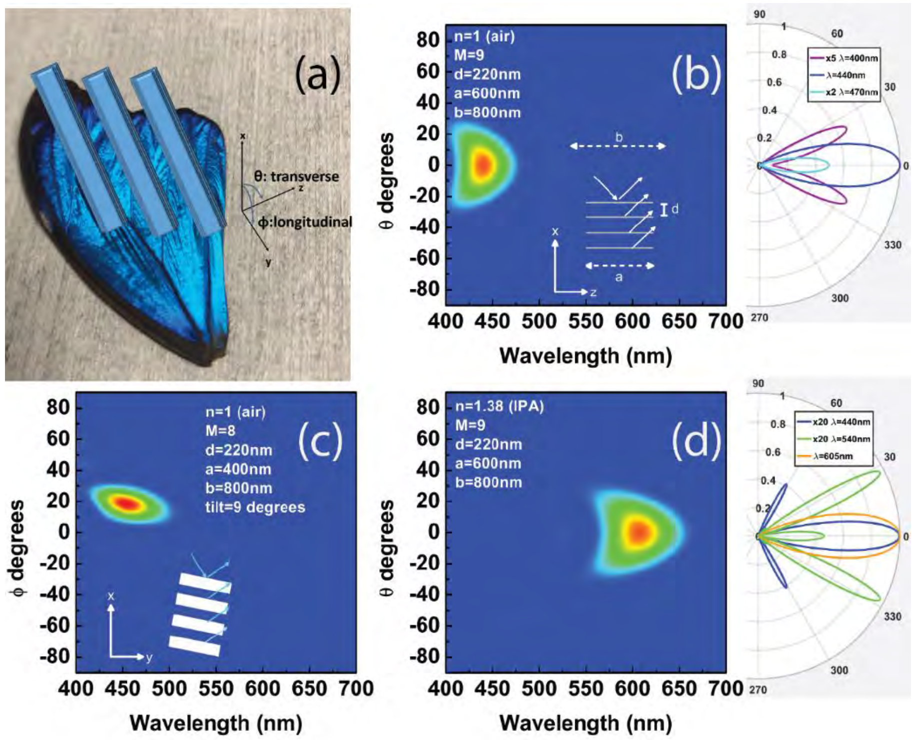


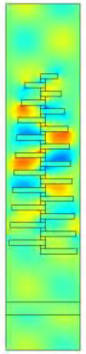




Thinking a butterfly wing as an antenna array

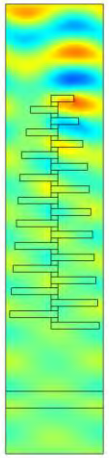




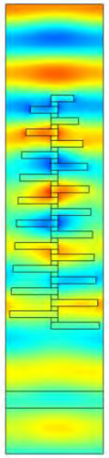


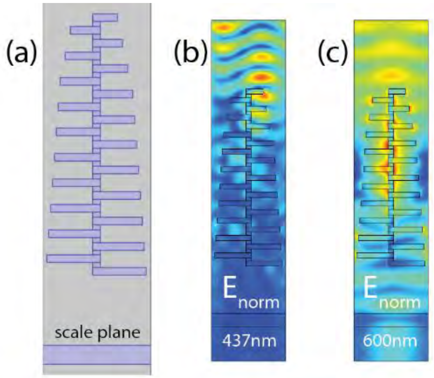
Thinking a butterfly wing as an antenna array

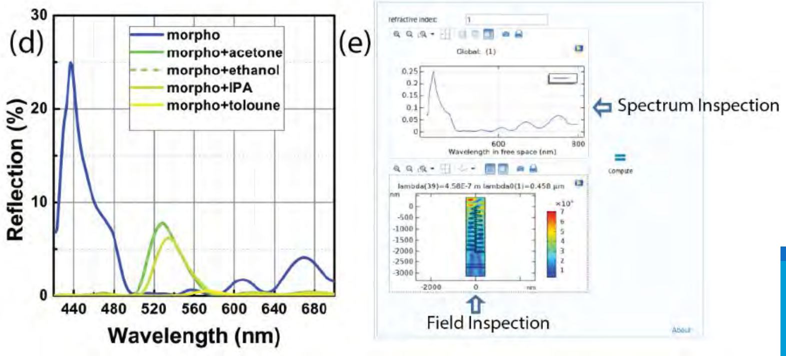
λ=437 nm *E* field *x* component

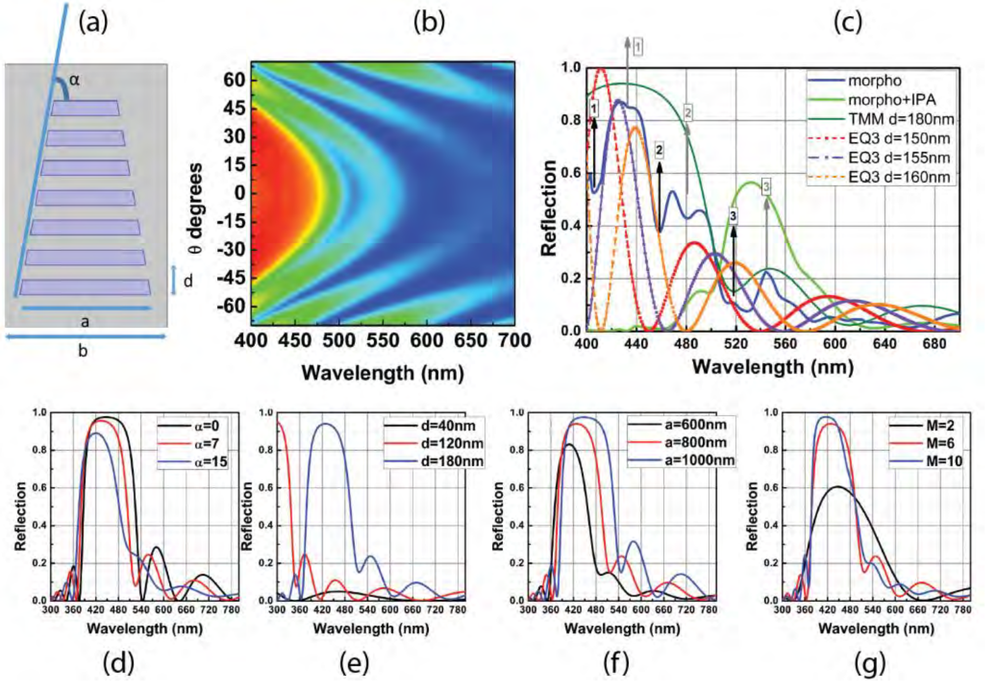


λ=600 nm *E* field *x* component









A sensor? More about it here: https://sid.onlinelibrary.wiley.com/doi/full/10.1002/jsid.1071

X-ray Photoelectron Spectroscopy

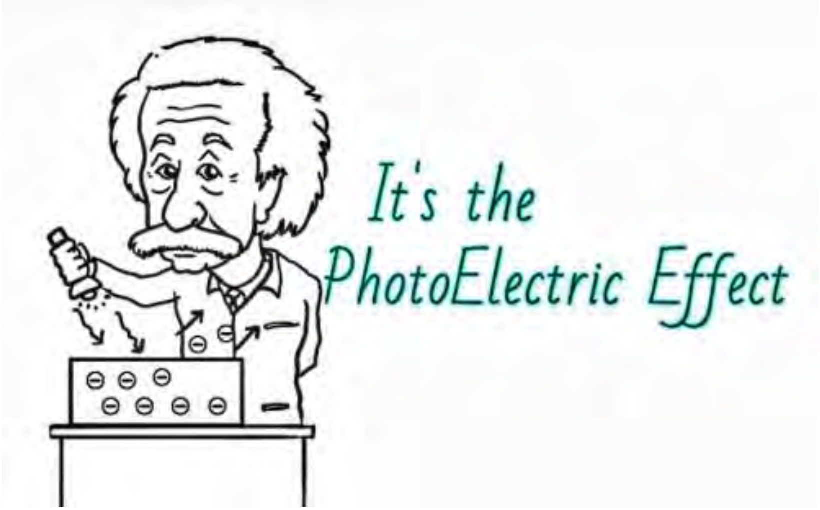
What is it and why is it important?

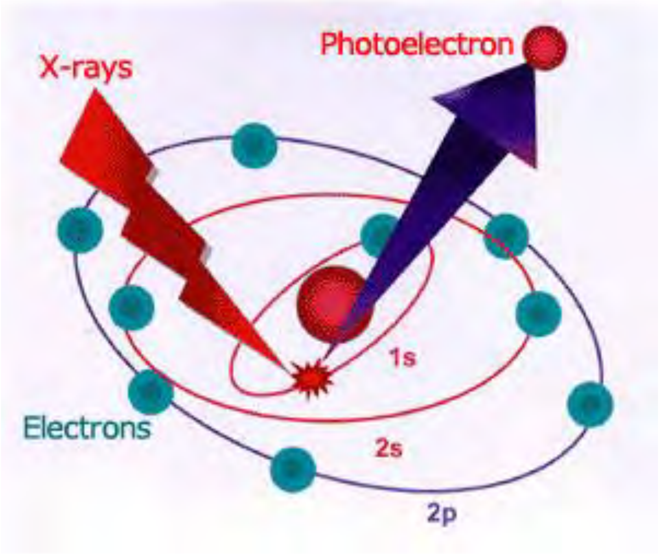
- Developed in 1960s as a surface analysis technique.
- Also known as Electron Spectroscopy for chemical analysis (ESCA).
- One of the most frequently used chemical analysis tool in order to determine
  - Elemental composition
  - Stoichiometry
  - Chemical state (e.g. oxidation state)
  - Electronic state of the elements

X-ray Photoelectron Spectroscopy

What is it and why is it important?

- Relies on the Photoelectric Effect: **Shining a torchlight on any surface splashes away some surface electrons** due to the acquired energy from the incident light.





The Nobel Prize in Physics 1921 was awarded to Albert Einstein "for his services to Theoretical Physics, and especially for his discovery of the law of the photoelectric effect."

https://www.nobelprize.org/prizes/physics/1921/summary/

Photoelectron Spectrometer (ESCA) | Introduction to JEOL Products | JEOL Ltd.

X-ray Photoelectron Spectroscopy

Examining the Photoelectric Effect

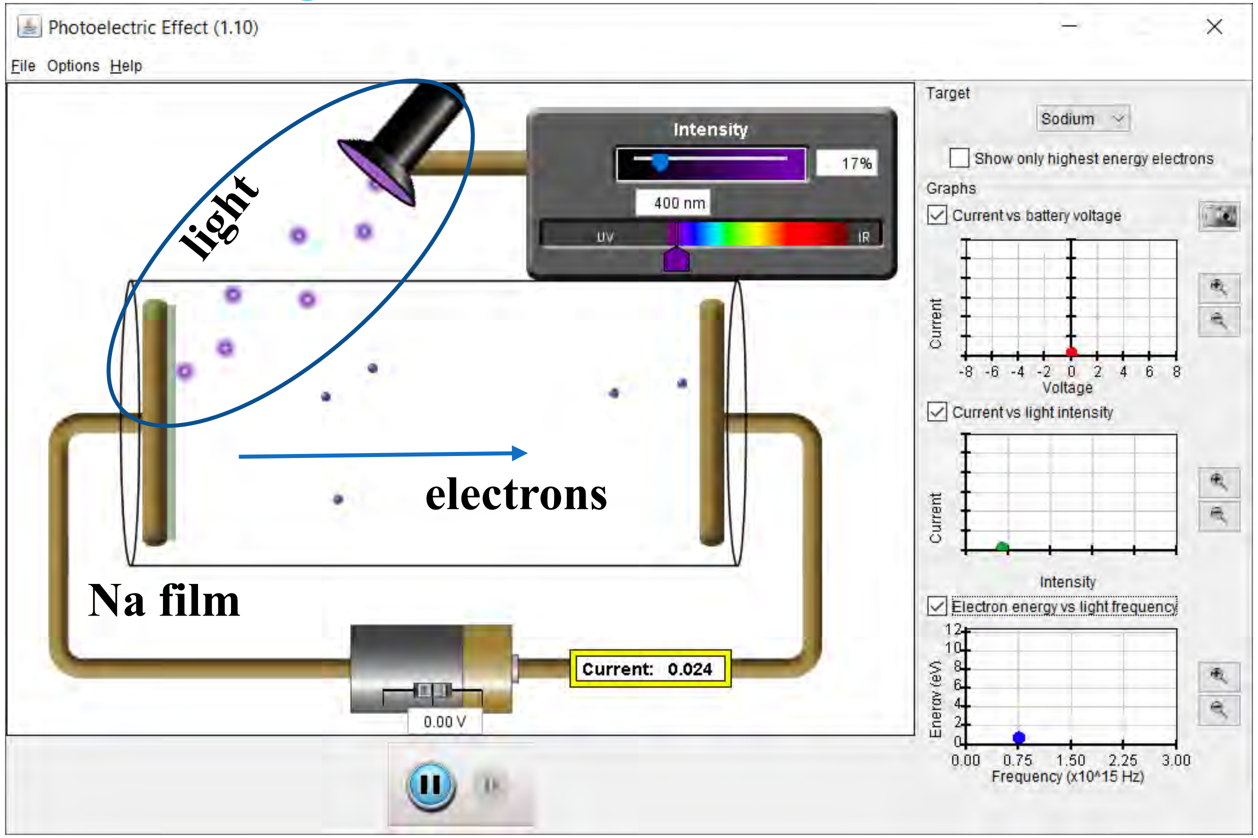
- Phet University of Colorado Boulder offers excellent simulations on Photoelectric Effect - Light | Quantum Mechanics | Photons - PhET Interactive Simulations (colorado.edu)
- Explore the rest of the simulation APPs here: Browse - PhET Interactive Simulations (colorado.edu)

PhET INTERACTIVE SIMULATIONS™

University of Colorado Boulder

X-ray Photoelectron Spectroscopy

Examining the Photoelectric Effect



Case1: Illuminating Na (Sodium)

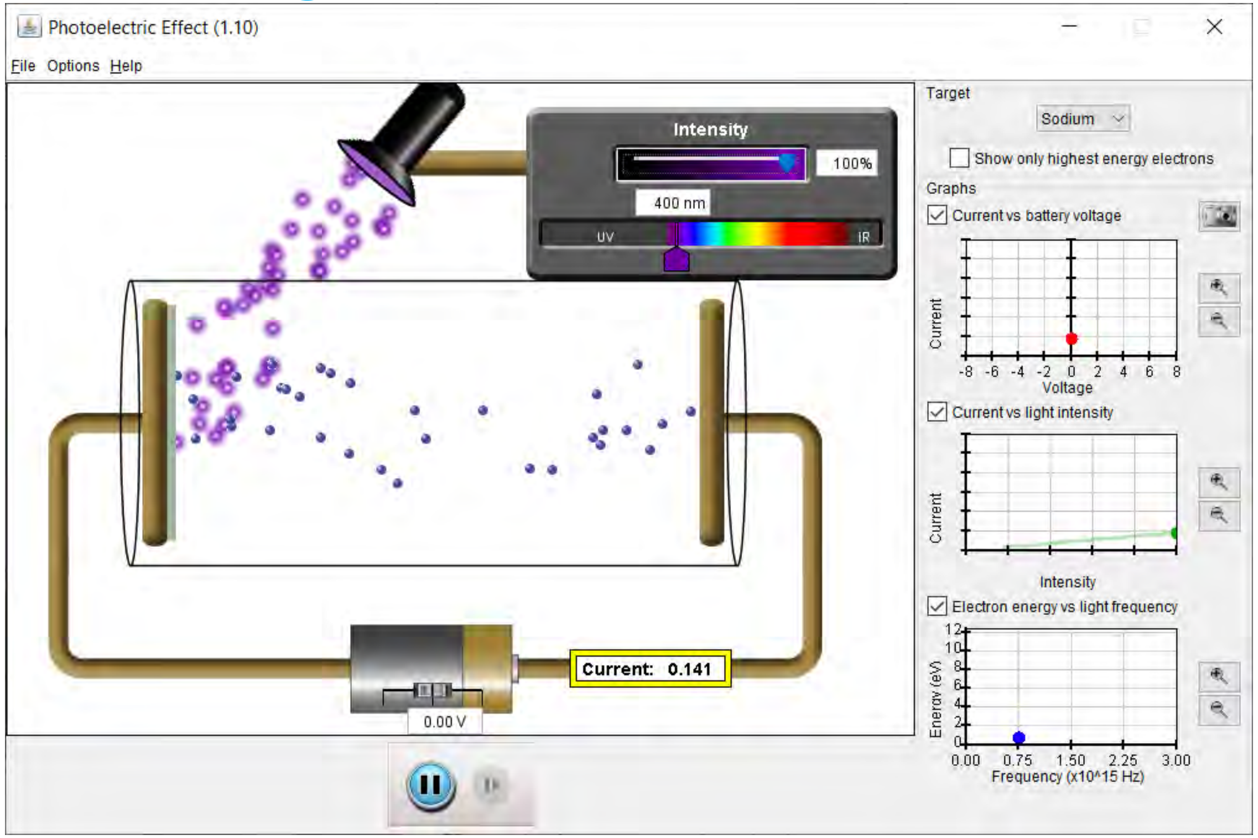
Light impinges on a thin Na film.

Electrons are extracted thanks to the illumination at **400nm wavelength with 17% intensity**.

Displaced electrons go to the other electrode and **yield current conduction of 0.024 Amperes**.

X-ray Photoelectron Spectroscopy

Examining the Photoelectric Effect



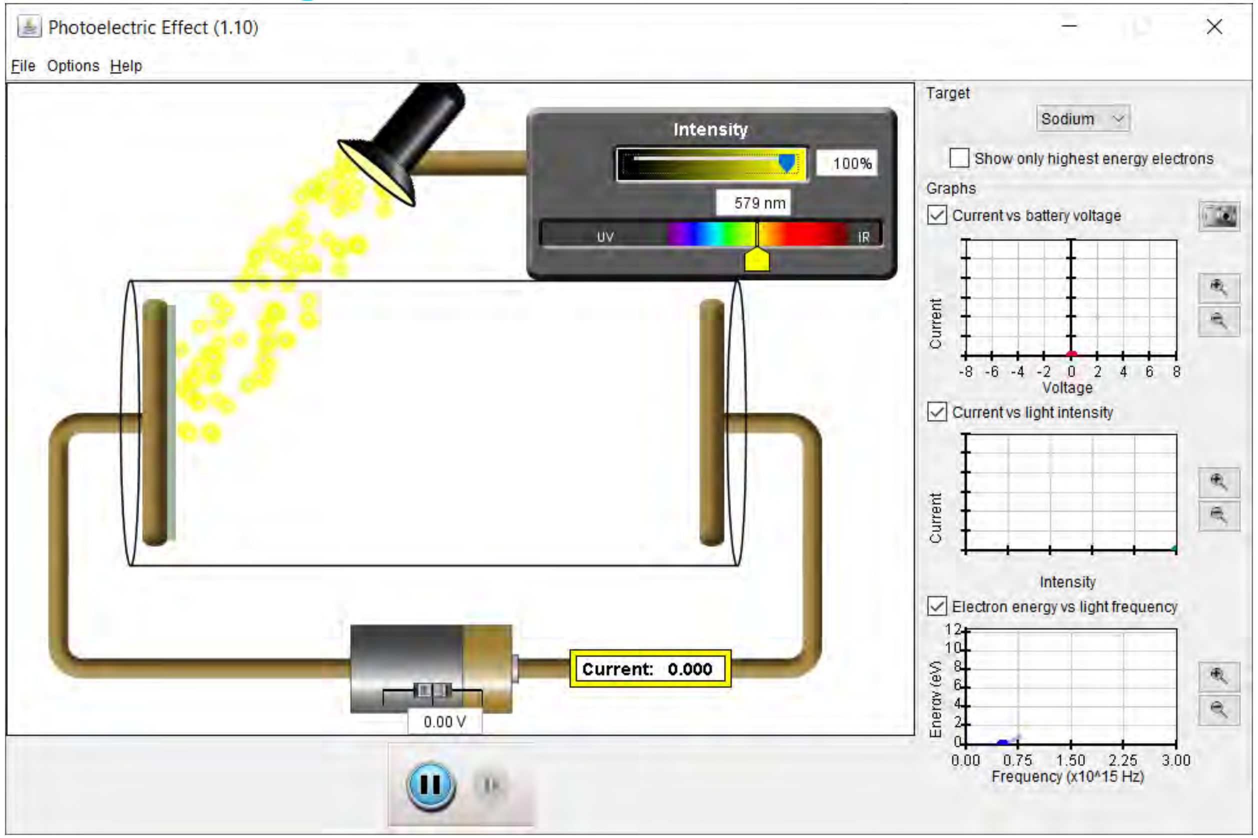
Case1: Illuminating Na (Sodium)

Increased intensity to 100% **yields more electrons** to be extracted. Thereby more current reading by the students. More photons impinging on the Na film extracts more electrons.

More Intensity => More Light => More Electrons Extracted => More Current

X-ray Photoelectron Spectroscopy

Examining the Photoelectric Effect



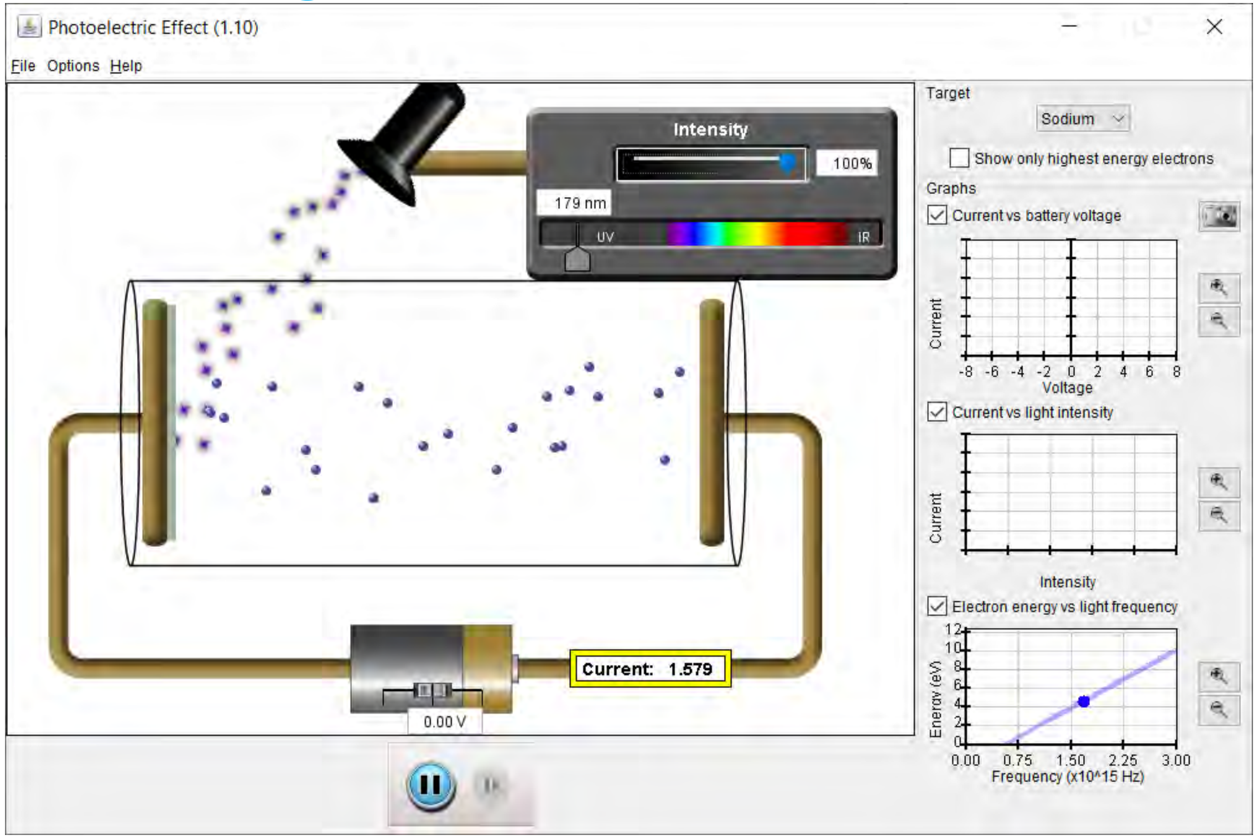
Case1: Illuminating Na (Sodium)

Increasing the wavelength of impinging light to 579nm. There is **no electron extraction!** Higher wavelength of light possesses lower energy, hence less or no electrons are extracted.

Higher Wavelength => Less Energy of Light => Less or No Electrons Extracted => Less or No Current

X-ray Photoelectron Spectroscopy

Examining the Photoelectric Effect



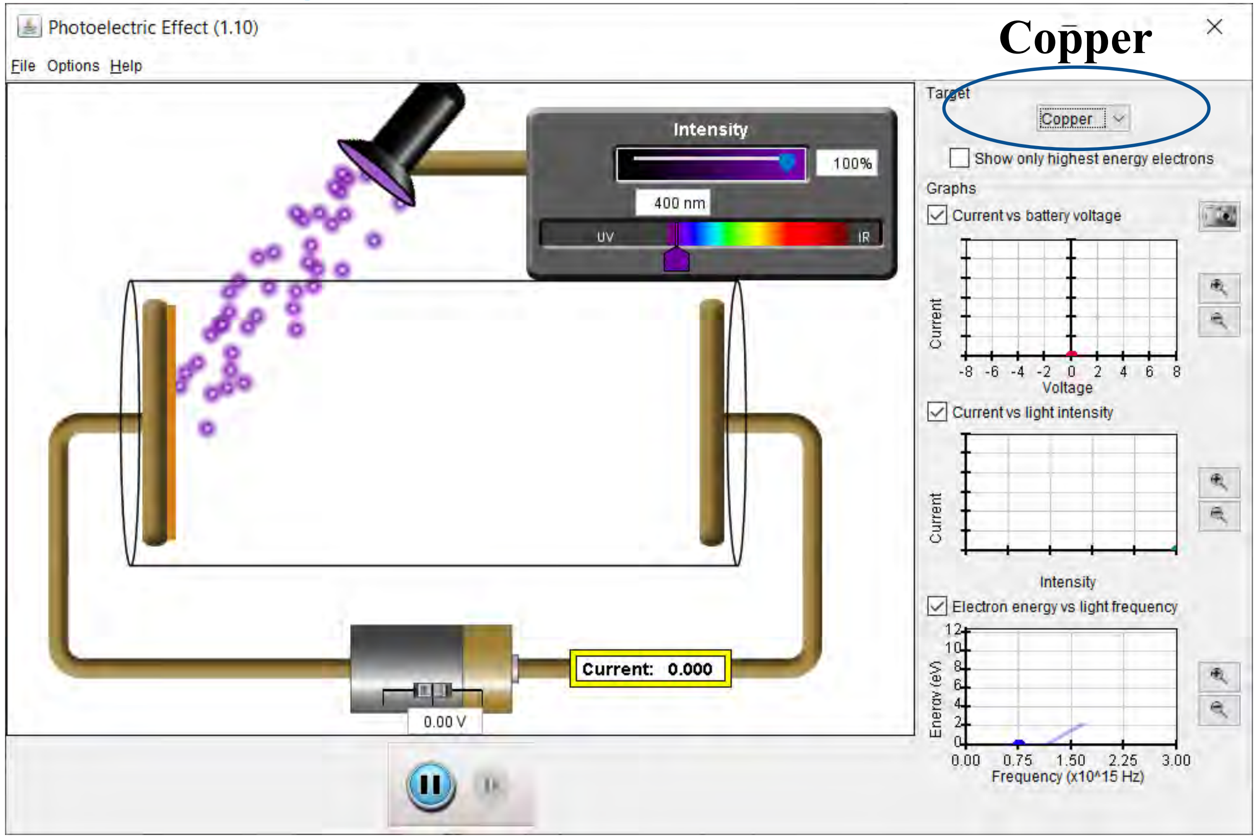
Case1: Illuminating Na (Sodium)

Opposite is also *generally* true (there are secondary effects outside of the scope). **More energetic, compare speed with 1st case, wavelength 400nm!**

Lower wavelength => Higher Energy of Light => More Electrons Extracted => More Current

X-ray Photoelectron Spectroscopy

Examining the Photoelectric Effect



Case2: Illuminating Cu (Copper)

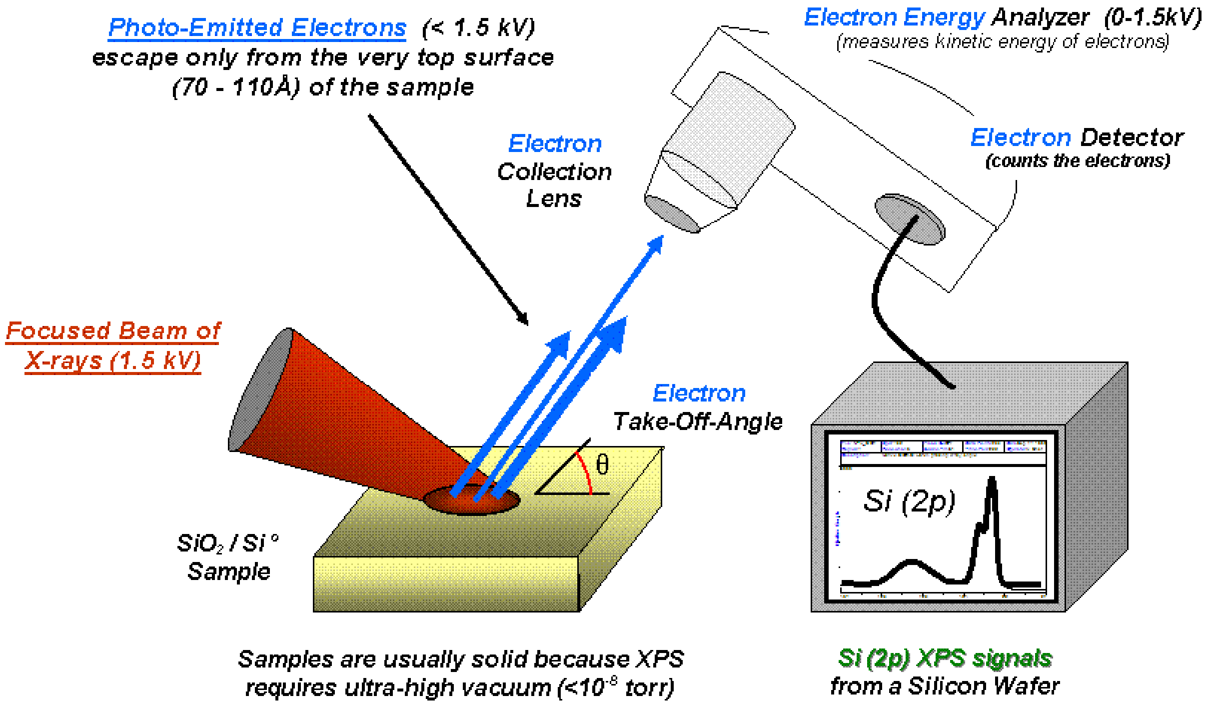
At wavelength of 400nm, Cu does not yield any current. No electrons extracted. **Cu has higher atomic number (Z) and requires higher energy** to extract the electrons.

In other words, Cu has higher **binding energy** (E_B)!

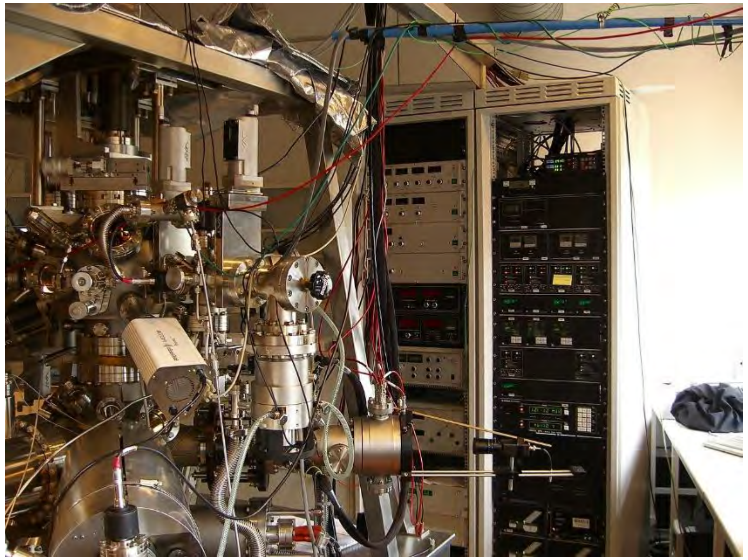
X-ray Photoelectron Spectroscopy

XPS tool and exposure for the students

Illuminating the surface with x-rays to extract core electrons to fulfill an elemental analysis. Might be challenging to give the exposure to the students with limited funds.



Images taken from Wikipedia



X-ray Photoelectron Spectroscopy

XPS tool and exposure for the students

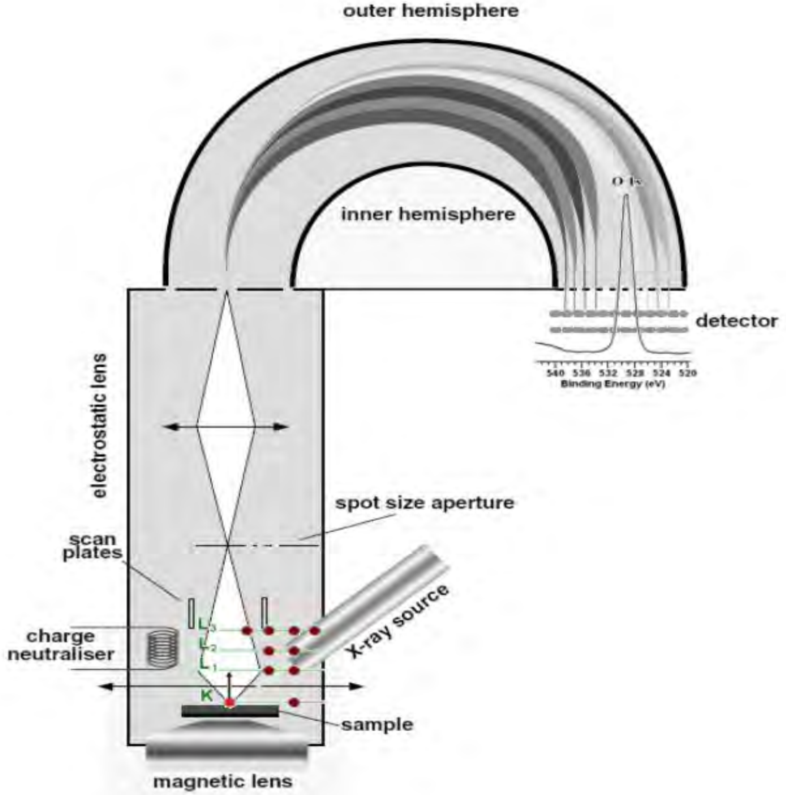


Image taken from Teignmouth Science and Technology Center

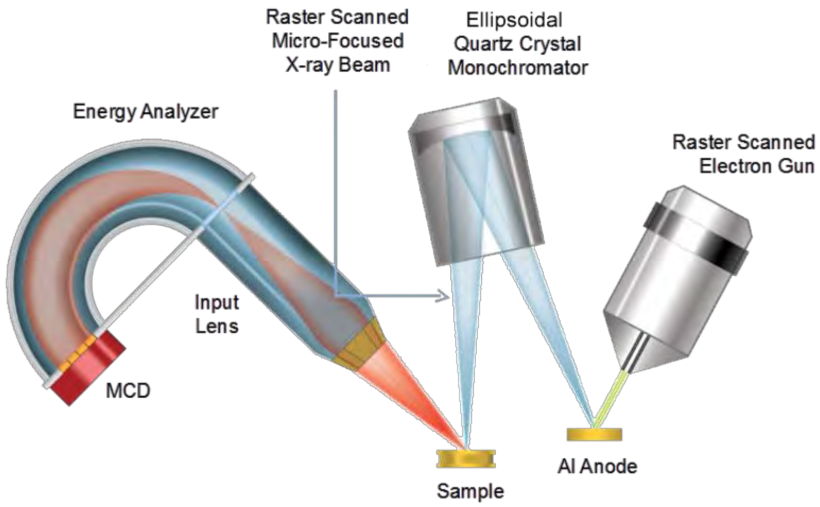


Image taken from X-Ray Photoelectron Spectroscopy (XPS) Surface Analysis Technique (phi.com)

A modern XPS operating under Ultra High Vacuum with an X-ray source generally emitted from Al or Mg anodes after receiving e-beam emission (from a Tungsten or LaB_6) filament. Quartz Monochromator produces a thin X-ray line width. Hemispherical sector analyzer with an electron lens are employed on the receiver side. Charge neutralizer might be needed for charging problems.

X-ray Photoelectron Spectroscopy

SESSA: Simulation of the Electron Spectra for Surface Analysis

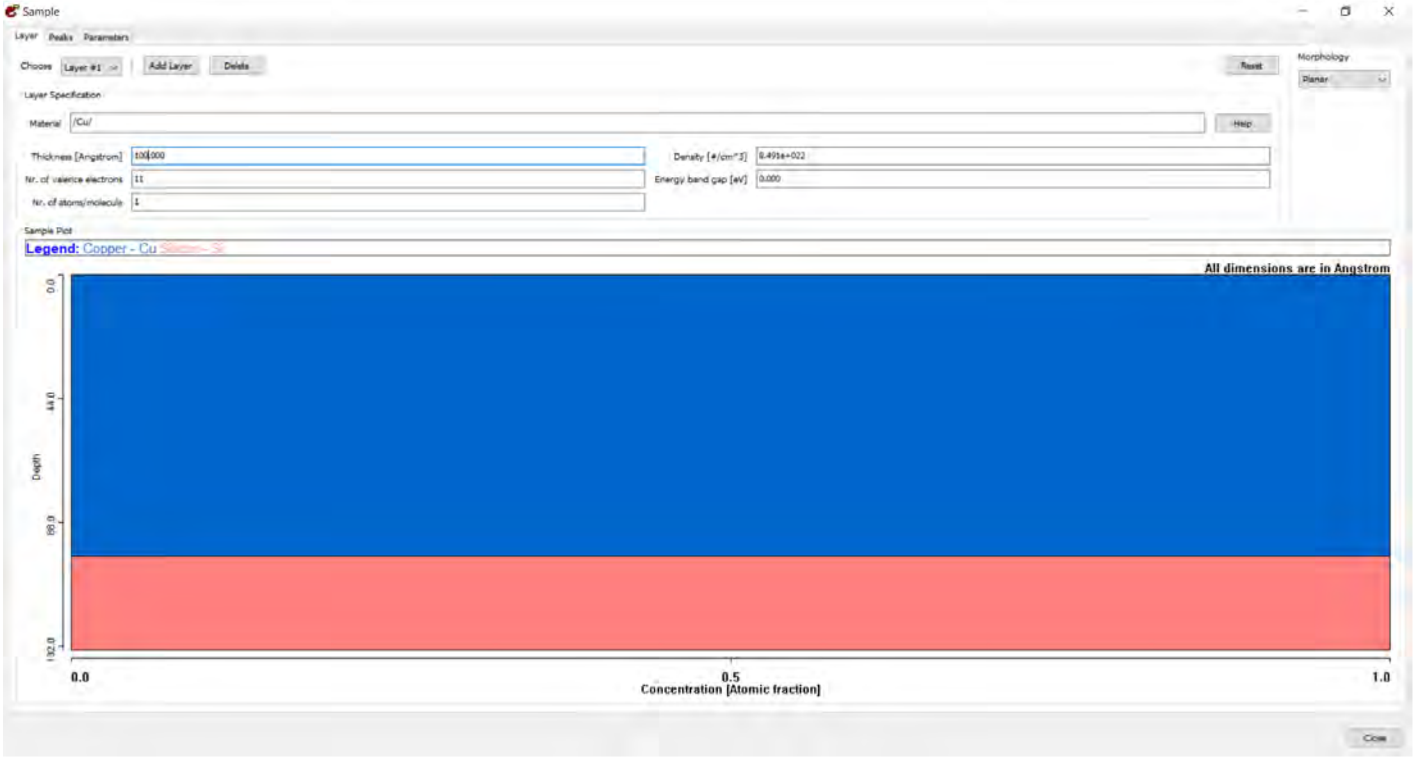
- Go to NIST Standard Reference Database 100 | NIST to download the proper version to your computer.

NIST National Institute of Standards and Technology U.S. Department of Commerce

X-ray Photoelectron Spectroscopy

SESSA Exercise1: Cu survey result

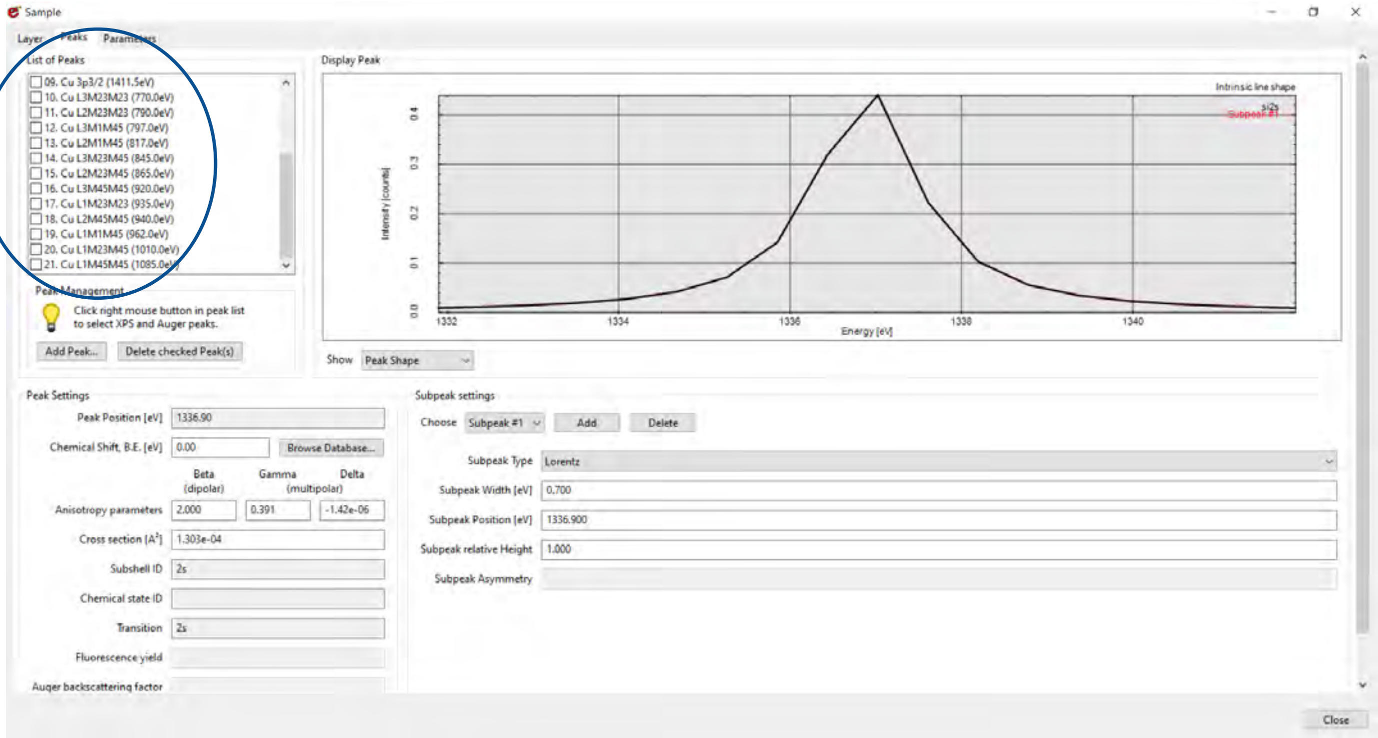
- Set up a 10nm (thick) Cu layer on Si substrate from Sample tab.



X-ray Photoelectron Spectroscopy

SESSA Exercise1: Cu survey result

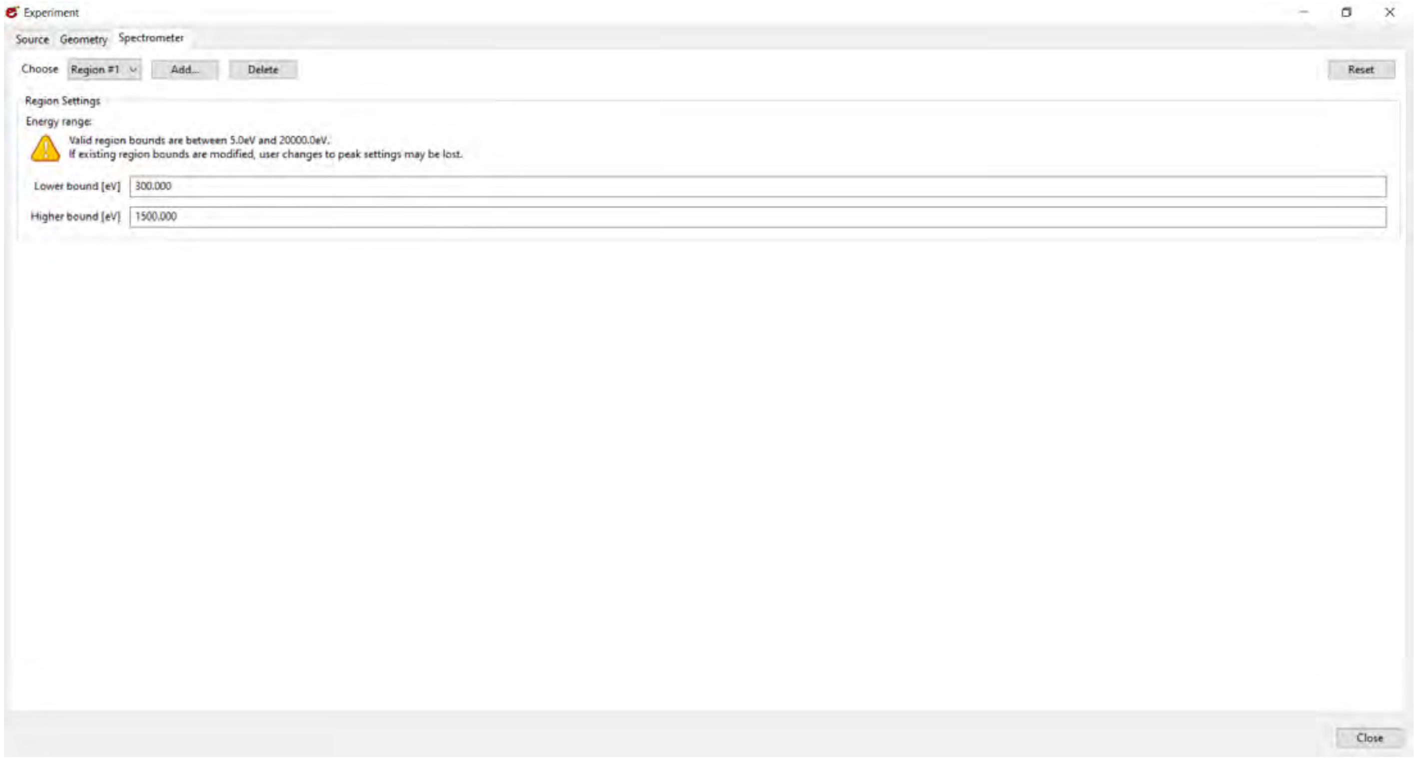
- Go to Peaks tab, you will see that there are various Auger peaks, aside from the XPS peaks.



X-ray Photoelectron Spectroscopy

SESSA Exercise1: Cu survey result

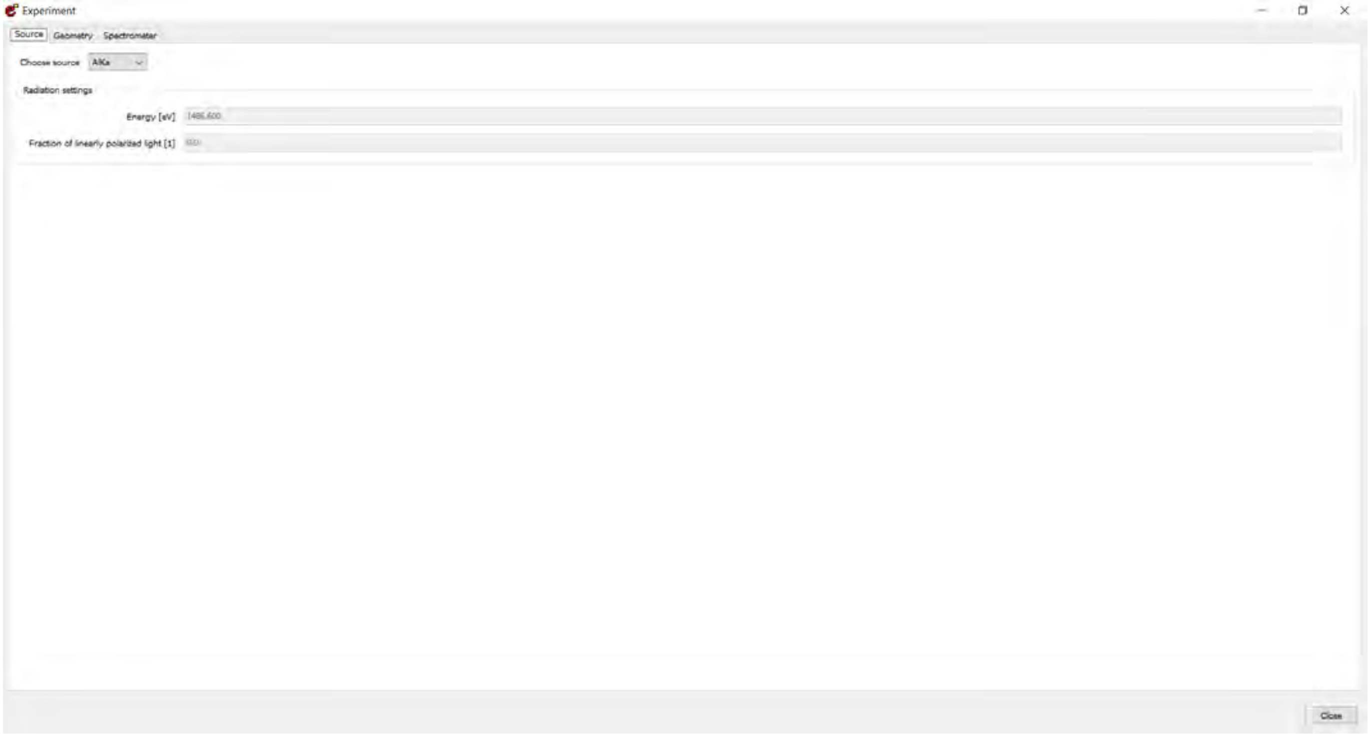
- Go to Spectrometer and set the lower and upper boundaries as 300eV and 1.2keV, respectively.



X-ray Photoelectron Spectroscopy

SESSA Exercise1: **Cu survey result**

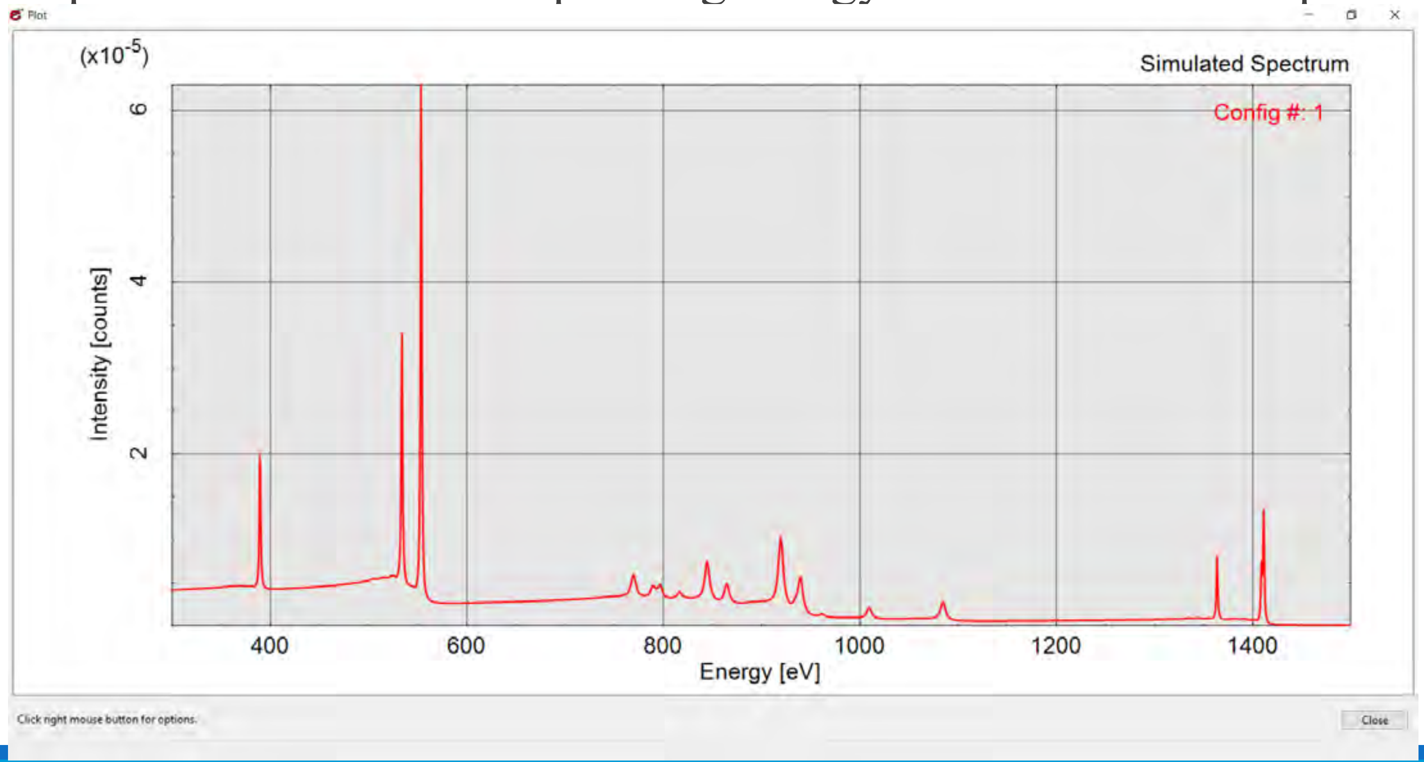
- Go to Source and observe the incident X-ray source, which is an AlKα source with an incident energy (E_i) of 1486eV.



X-ray Photoelectron Spectroscopy

SESSA Exercise1: Cu survey result

- Go to Simulation tab and hit Start Simulation, you should obtain the following plot. Students can extract the peak values and corresponding energy values with the help of the mouse.



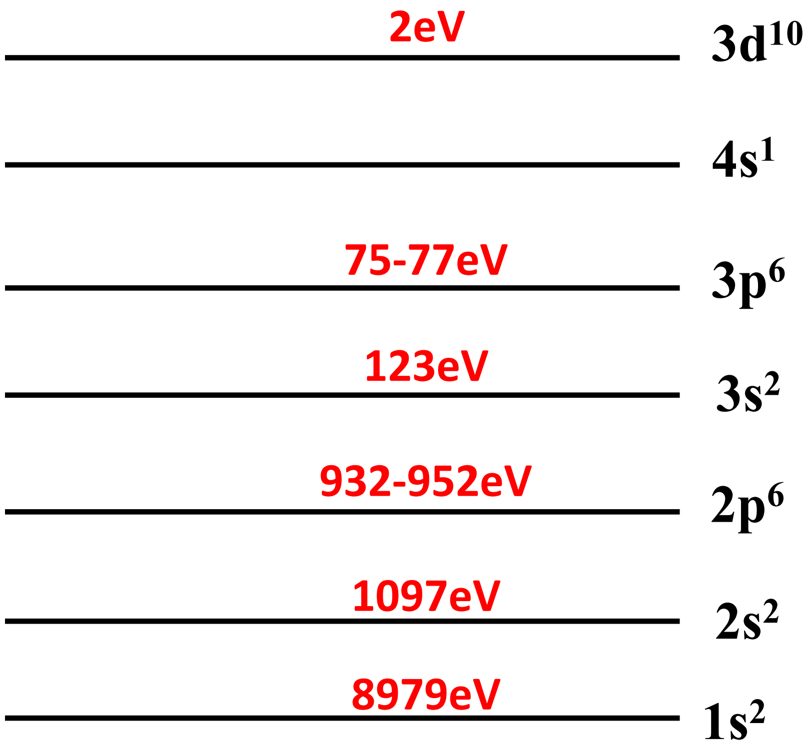
X-ray Photoelectron Spectroscopy

SESSA Exercise1: Cu survey result

- Referring back to the Periodic Table, Cu can be arranged as:

  $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^{10}$

Image taken from [Copper – The Element We can Count on : Chemical Industry Digest (chemindigest.com)]

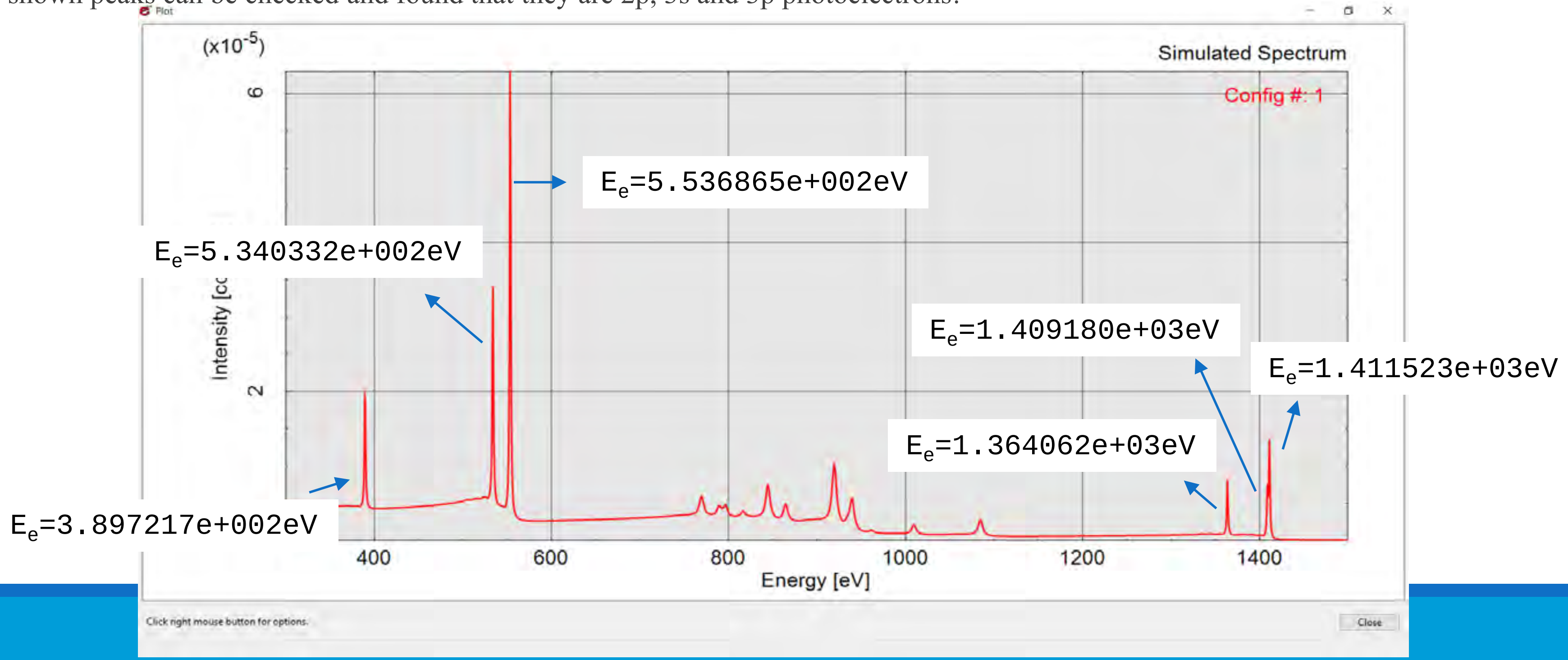


Red labeled energy values are the binding E_B values of the electrons.

X-ray Photoelectron Spectroscopy

SESSA Exercise1: **Cu survey result**

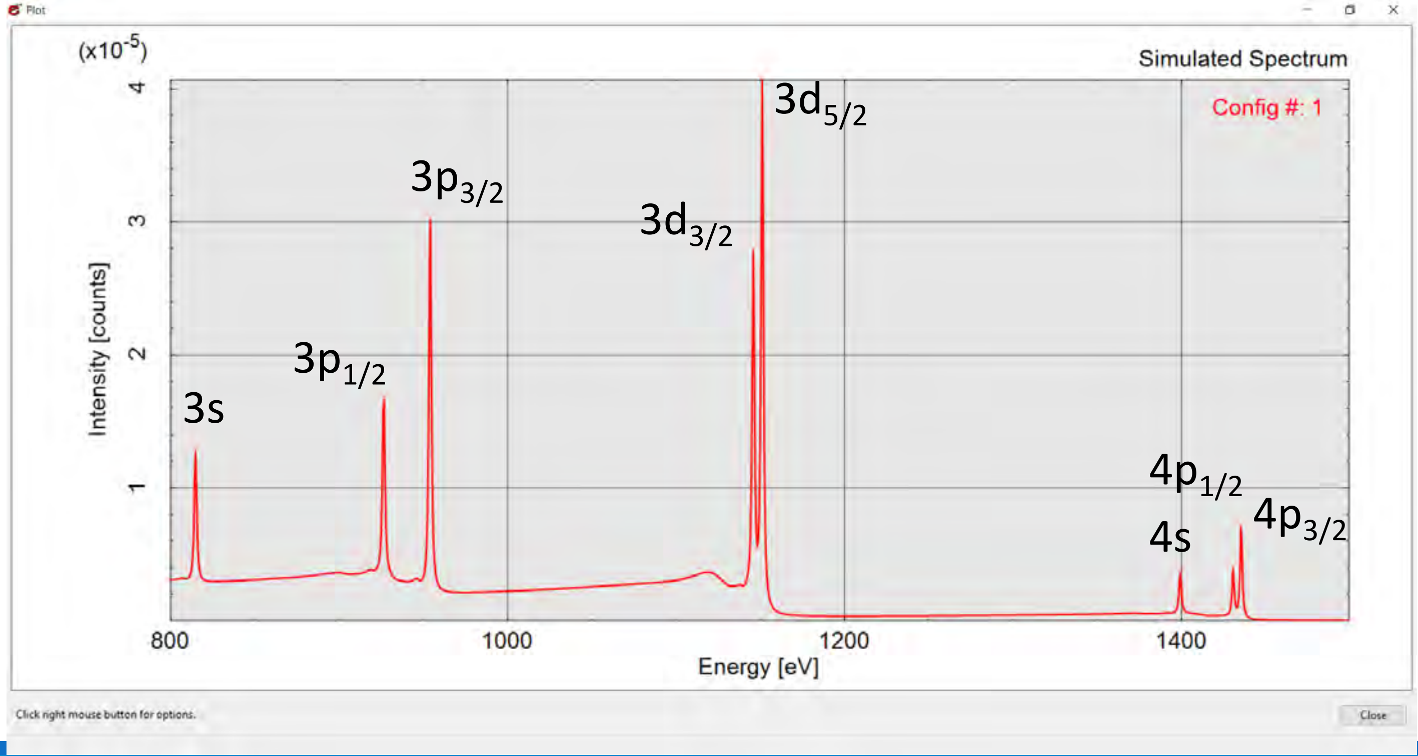
- Retrieved peaks (photoelectron Energy values) E_e and E_b values from the previous slide match? Energy should be conserved.
  - 1st peak => $E_e=E_i- E_b$ => 1486eV-1097eV=389eV => This is 2s photoelectron!
  - Other shown peaks can be checked and found that they are 2p, 3s and 3p photoelectrons!



X-ray Photoelectron Spectroscopy

SESSA Exercise2: Pd survey result and spin-orbit splitting

- Follow similar steps for 10nm Pd instead of Cu and collect the results. Should collect 8 peaks. The peaks are associated with orbits.



X-ray Photoelectron Spectroscopy

SESSA Exercise2: Pd survey result and spin-orbit splitting

- Pd is a heavy atom with the dominant effect observed as L-S Coupling. More detailed reading can be found here: Angular Momentum Coupling (gsu.edu)

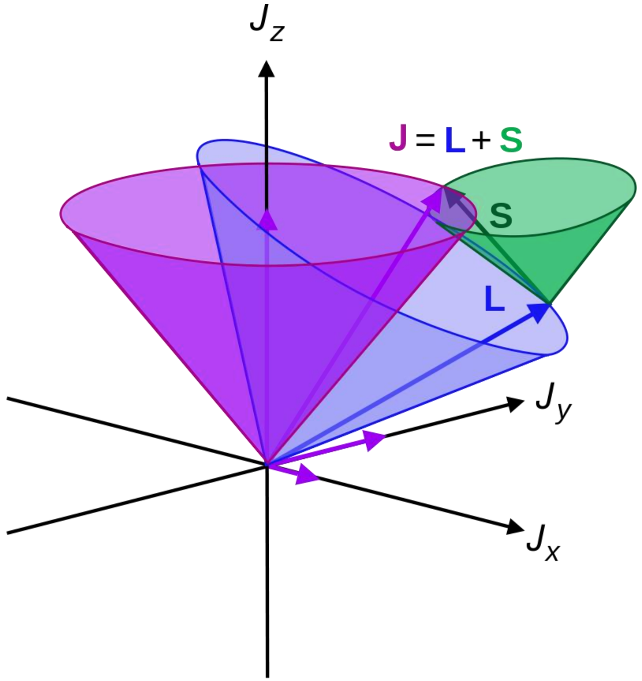


Image taken from Wikipedia

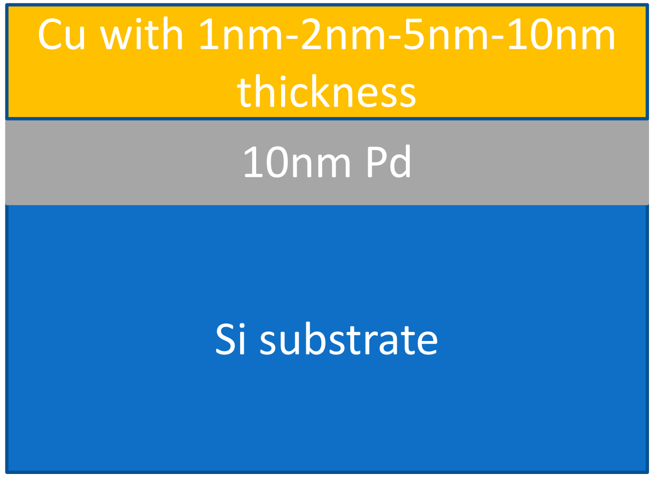
Inner core electron configuration is **$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10}$…** will remove an electron from 3d

Total Angular Momentum:
d orbit => L=2
S (spin)=1/2
|L-S| and |L+S| splitting will occur => $3d_{5/2}$ and $3d_{3/2}$
p orbit => L=1
S=1/2
|L-S| and |L+S| splitting will occur => $3p_{1/2}$ and $3p_{3/2}$

X-ray Photoelectron Spectroscopy

SESSA Exercise3: Escape length, mean free path and surface sensing.

- This exercise shows the surface sensing capability of XPS.
- On top of the Pd layer stack a Cu layer with changing thicknesses from 1nm, 2nm, 5nm to 10nm. We will quickly lose the peaks from Pd layer as the top Cu layer is getting thicker. The photoelectrons will not be able to escape the surface.



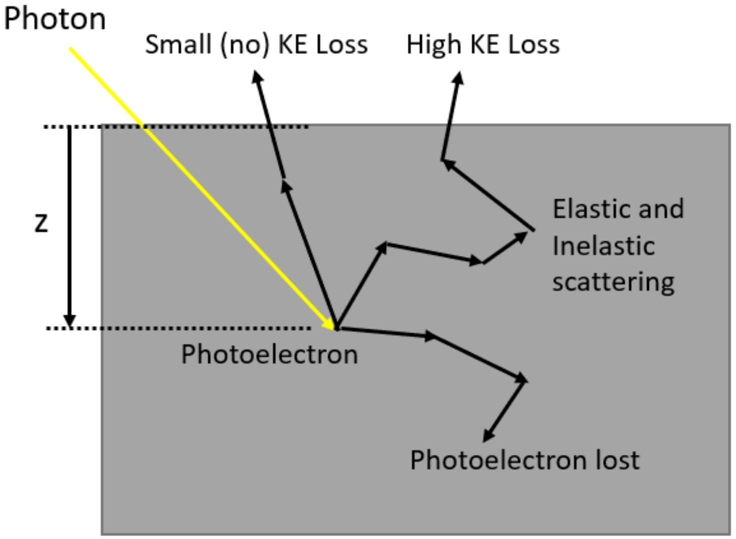
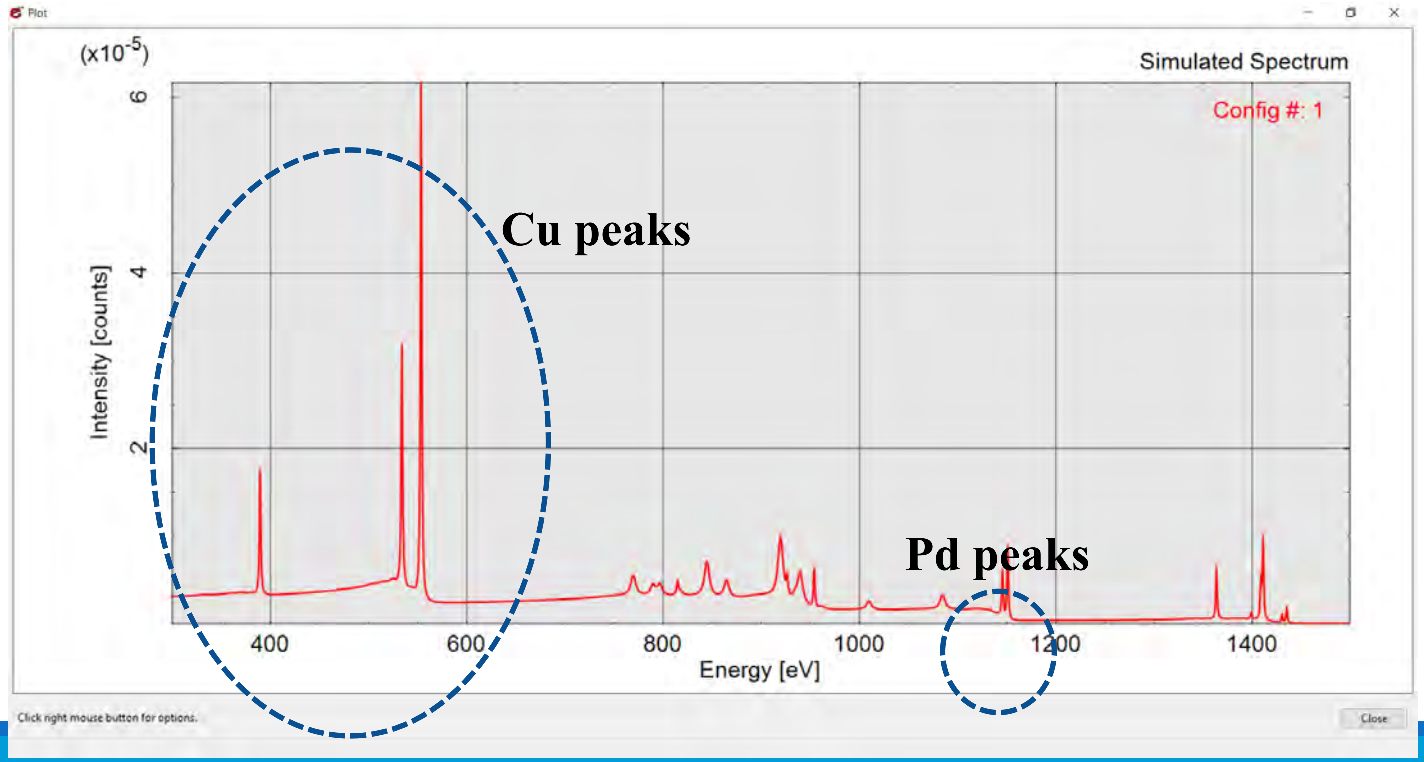


Image taken from Principles of XPS: Effective Attenuation Length

X-ray Photoelectron Spectroscopy

SESSA Exercise3: Escape length, mean free path and surface sensing.

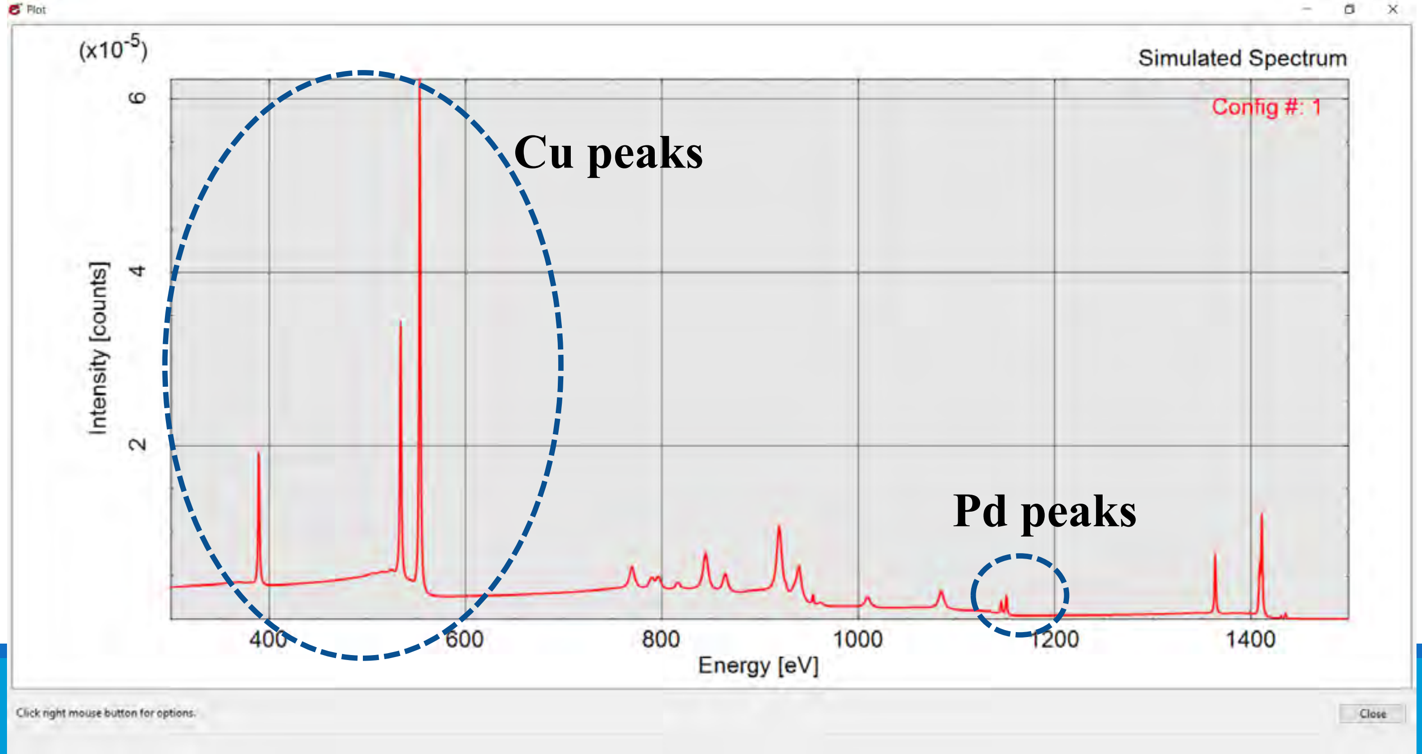
1nm Cu



X-ray Photoelectron Spectroscopy

SESSA Exercise3: Escape length, mean free path and surface sensing.

2nm Cu

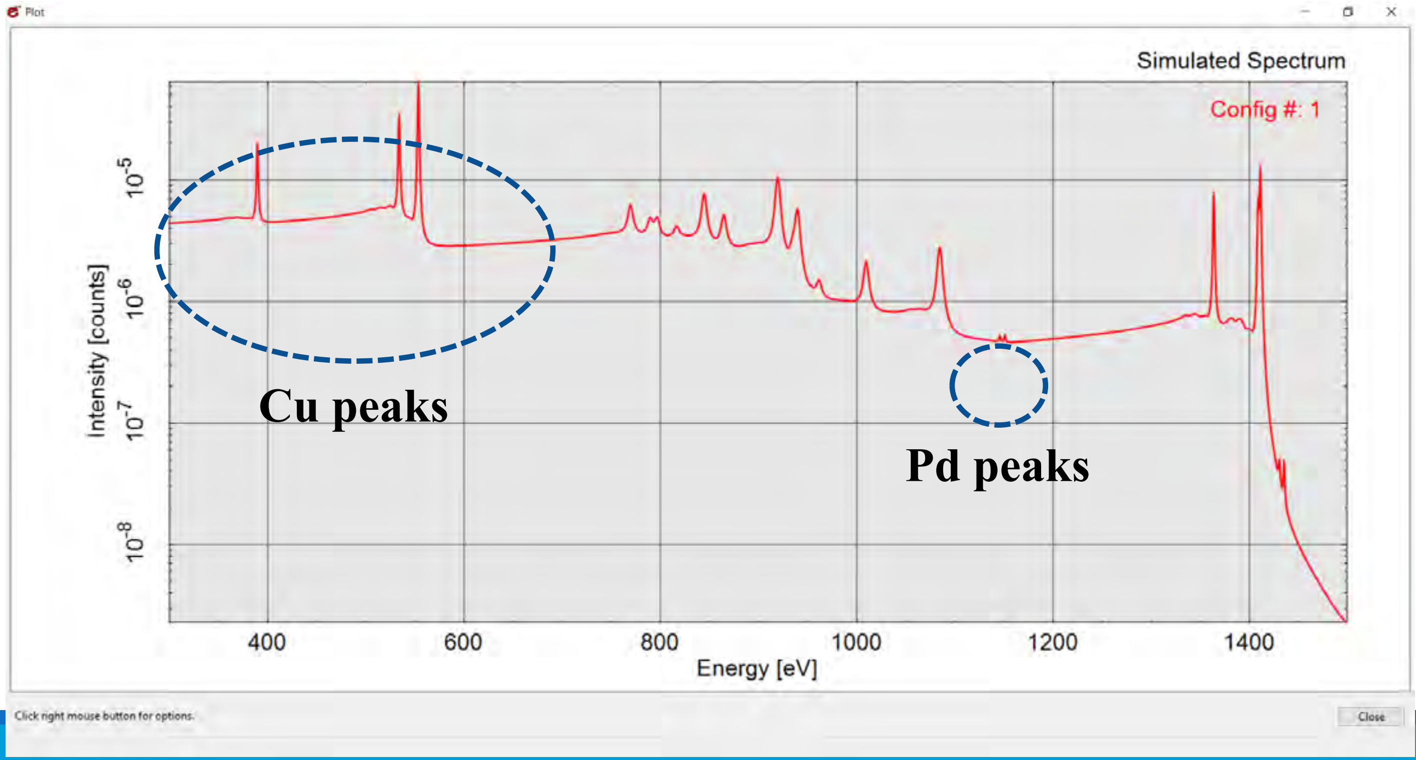


X-ray Photoelectron Spectroscopy

SESSA Exercise3: Escape length, mean free path and surface sensing.

- Plotting peaks in log scale

5nm Cu

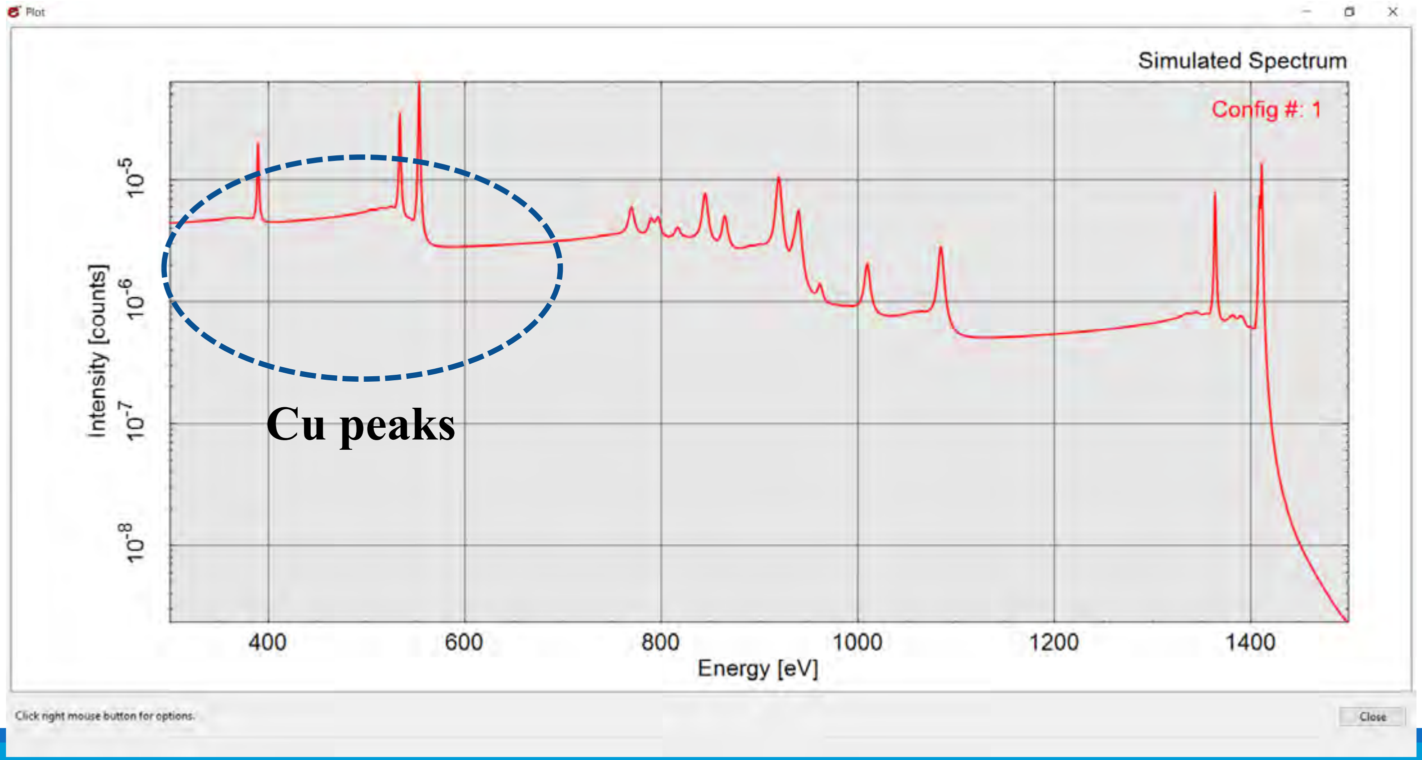


X-ray Photoelectron Spectroscopy

SESSA Exercise3: Escape length, mean free path and surface sensing.

- Plotting peaks in log scale

10nm Cu

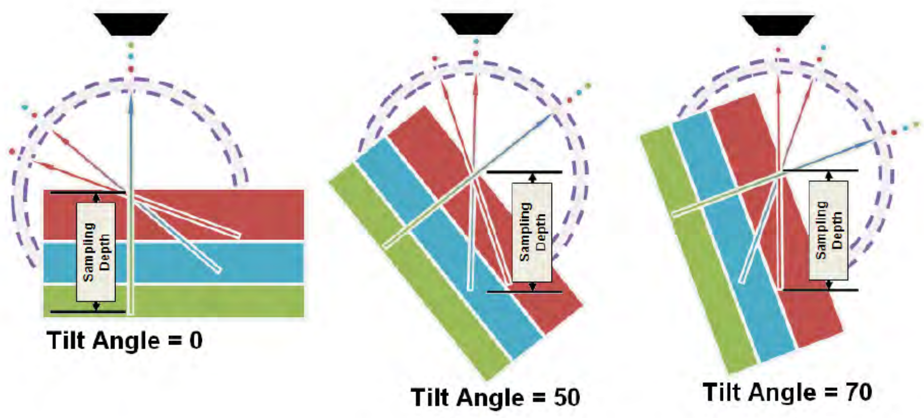


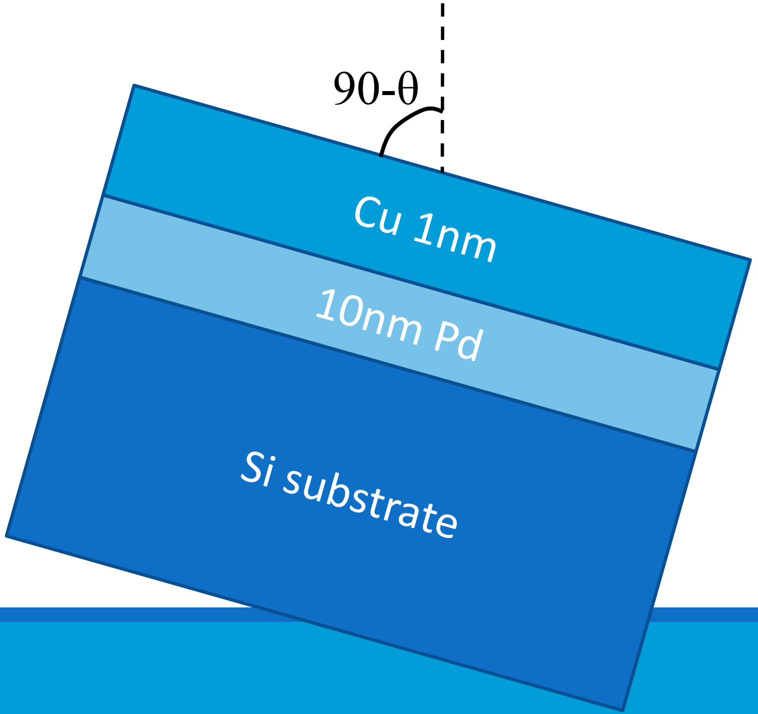
X-ray Photoelectron Spectroscopy

SESSA Exercise4: Depth Profiling

- Students can observe the sampling depth changes with the modifications done to the angle resolved XPS. The escape depth shrinks down with the tilted sample as schematically shown below.
- Change the tilt angle (Theta) from 0 to 30 to 60 degrees from Configurations tab.

Image taken from Teignmouth Science and Technology Center

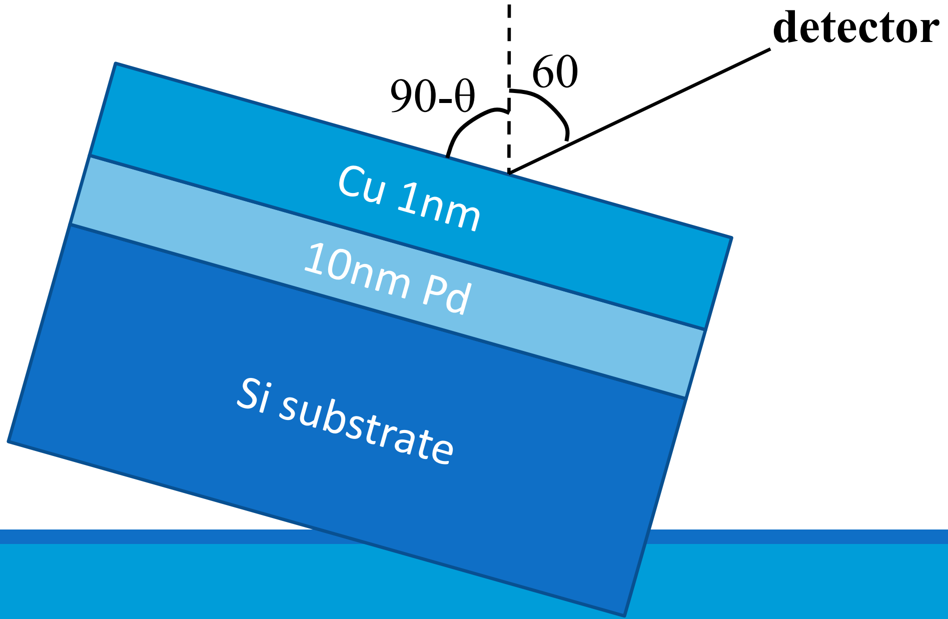




X-ray Photoelectron Spectroscopy

SESSA Exercise4: Depth Profiling

- Change the tilt angle (Theta) from 0 to 30 to 60 degrees from Configurations tab. Observe the changes in the signal intensity.
- Since the detector is already at a position with θ=60 degrees, the highest signal intensity will be collected from the underlying Pd layer when the sample is also tilted the same amount.

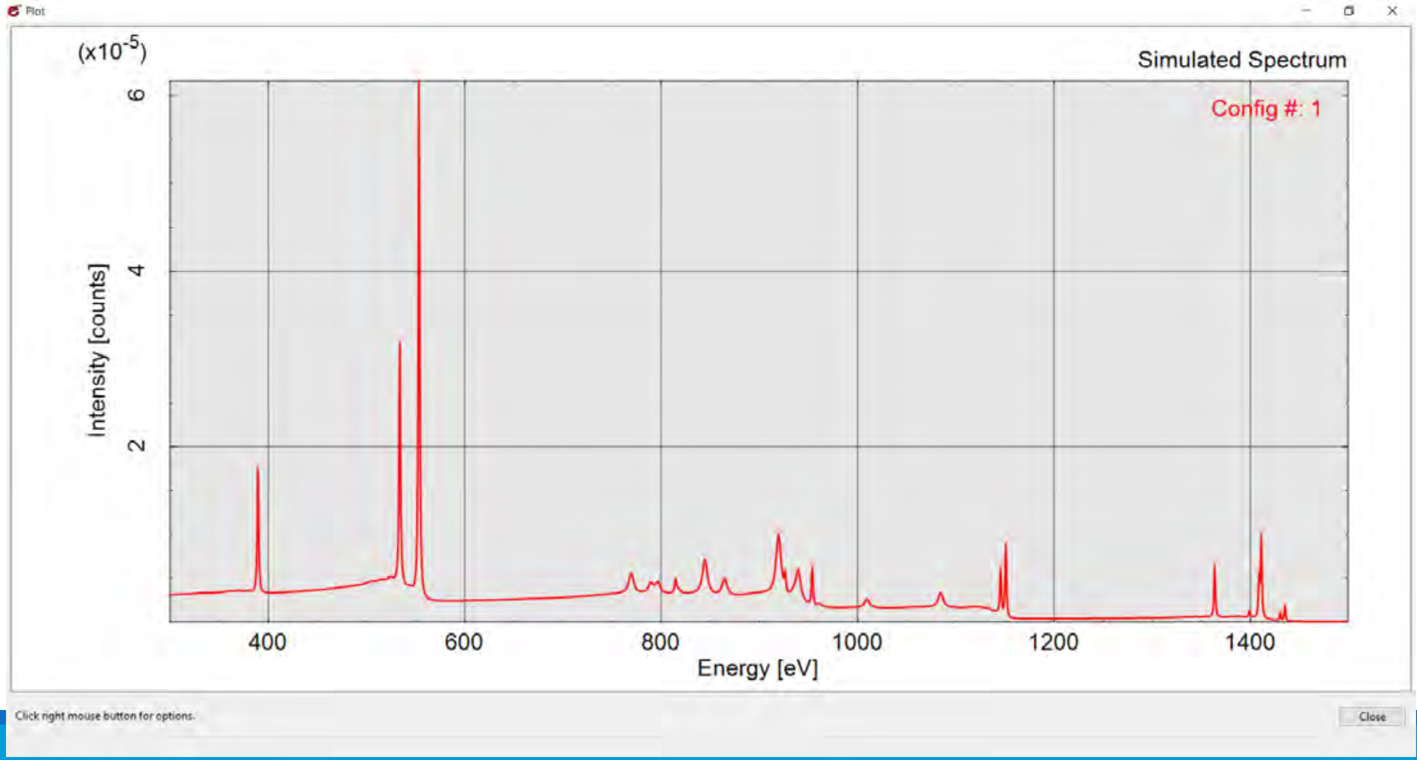


X-ray Photoelectron Spectroscopy

SESSA Exercise4: Depth Profiling

- Focusing on the Pd peaks only

θ=0 degrees

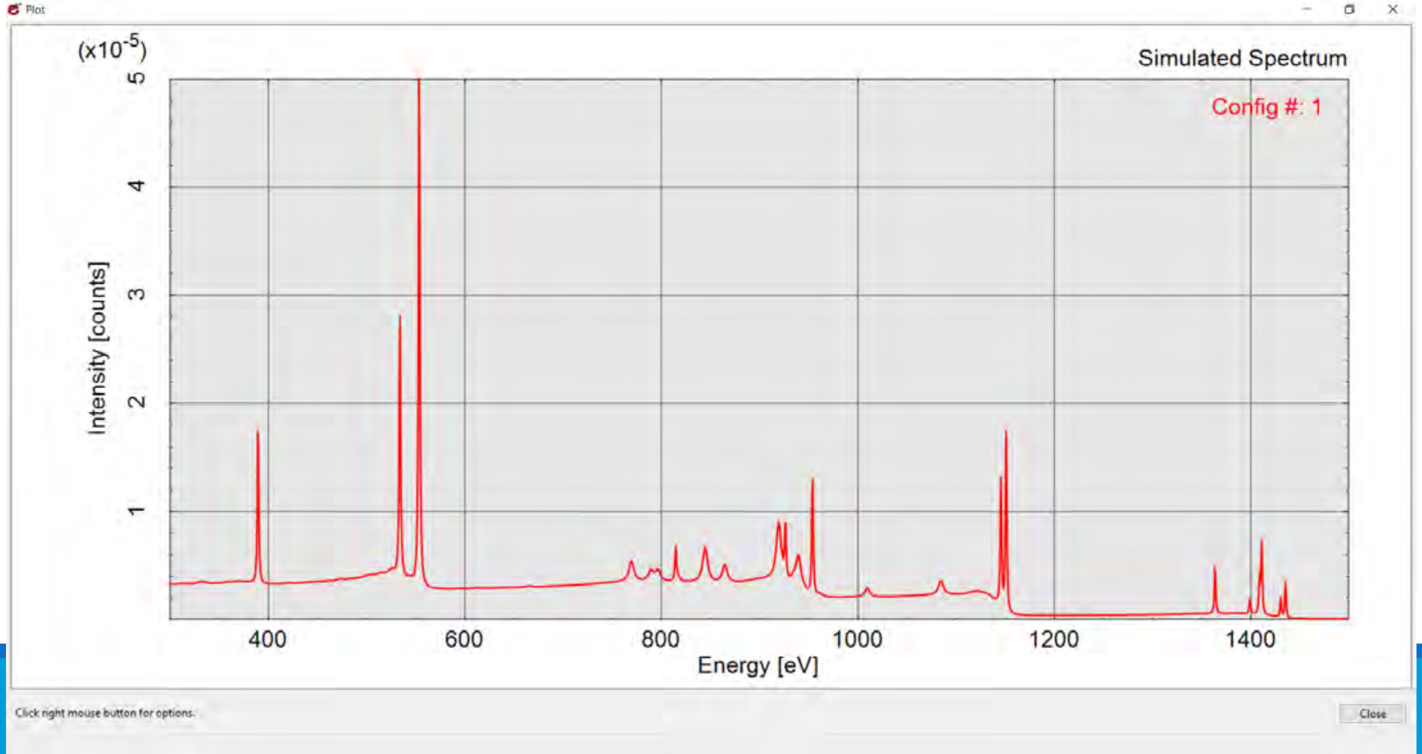


X-ray Photoelectron Spectroscopy

SESSA Exercise4: Depth Profiling

- Focusing on the Pd peaks only

θ=30 degrees

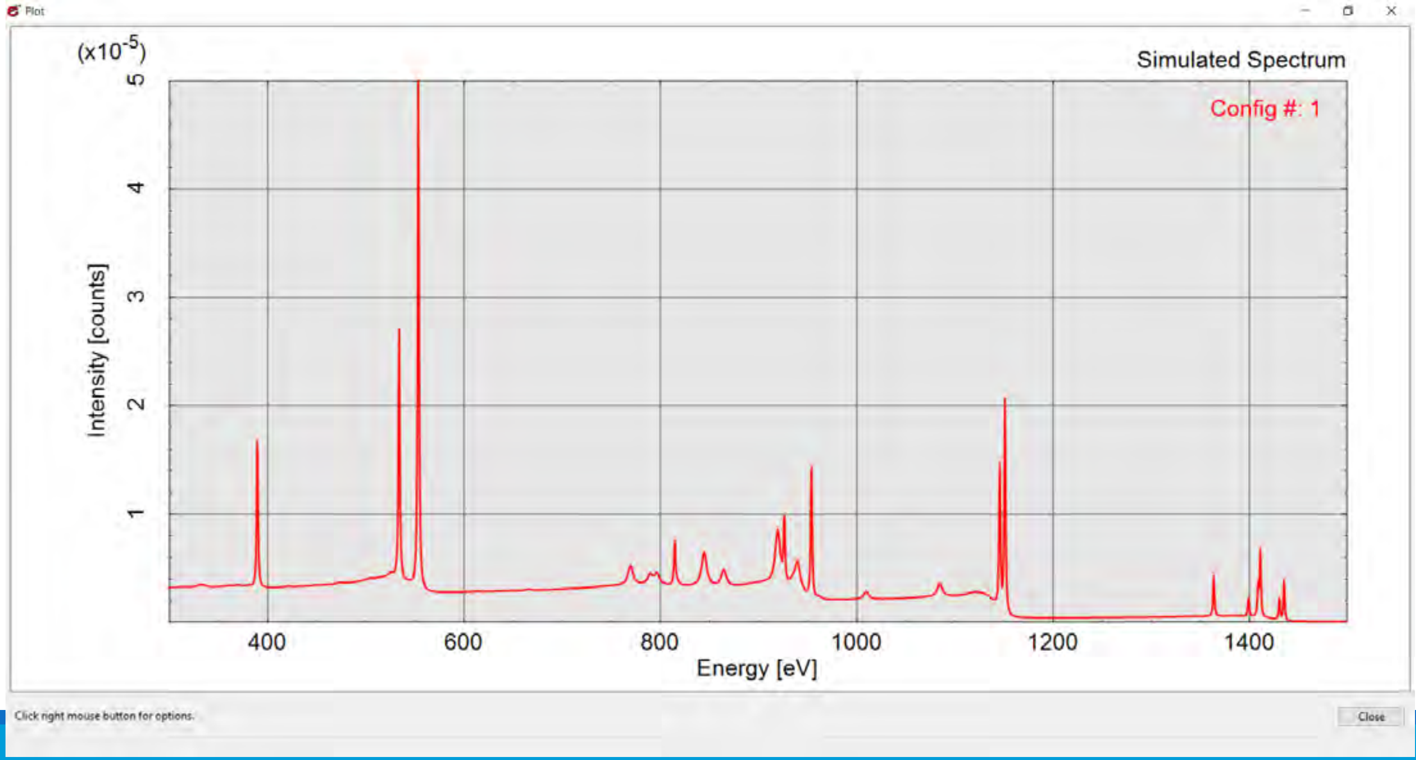


X-ray Photoelectron Spectroscopy

SESSA Exercise4: Depth Profiling

- Focusing on the Pd peaks only

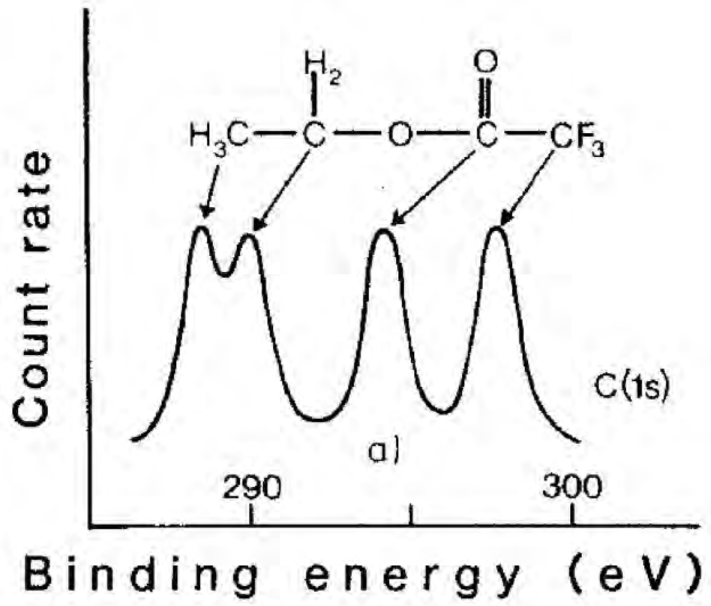
θ=60 degrees



X-ray Photoelectron Spectroscopy

SESSA Exercise5: Chemical Shift

- Students can observe the effect of the electronegativity on the binding energy as shown below for the same C atom binding to F as the most electronegative partner with the highest binding energy.



- Go to Sources tab and change the X-ray source to MgKα which is at E_i=1253.6eV
- We will observe the chemical shift as Si is oxidized.
- Go to Sample tab and change the material (single layer) to /Si[oxide]/O2/ for oxide

Si substrate

SiO_2 oxidized state

Image taken from Alessandro Kovtun's PhD thesis: 2D Graphene-based Materials. Interplay between Composition and Electrical Properties

X-ray Photoelectron Spectroscopy

SESSA Exercise5: **Chemical Shift**

- Go to the Peaks tab and under Si 2p peaks click on the Chemical Shift and choose a Good estimation peak for the O bonded Si.

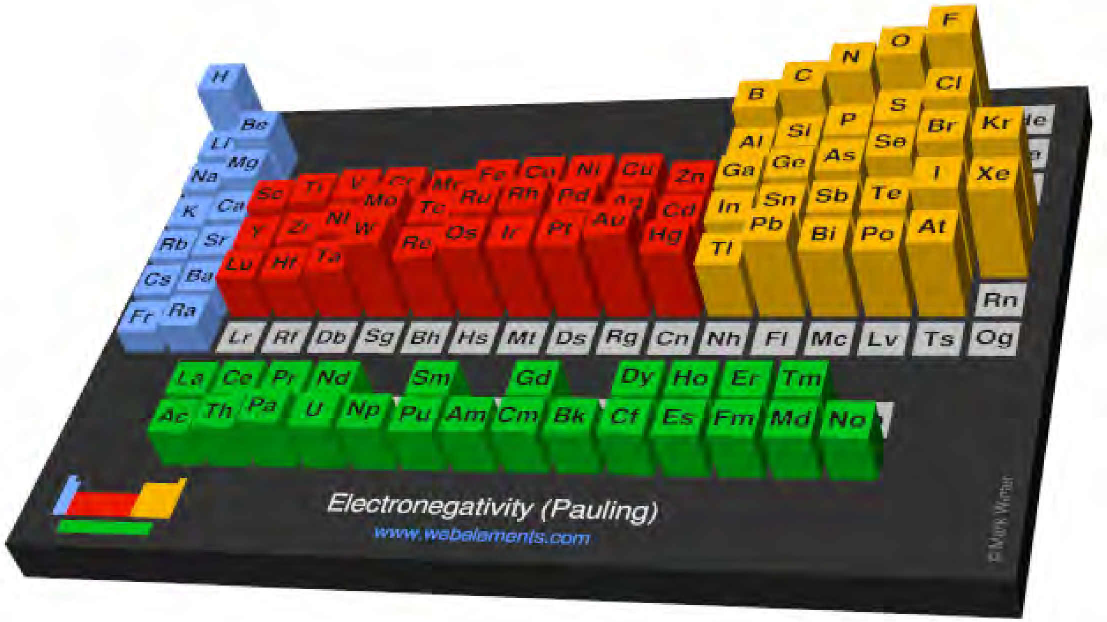
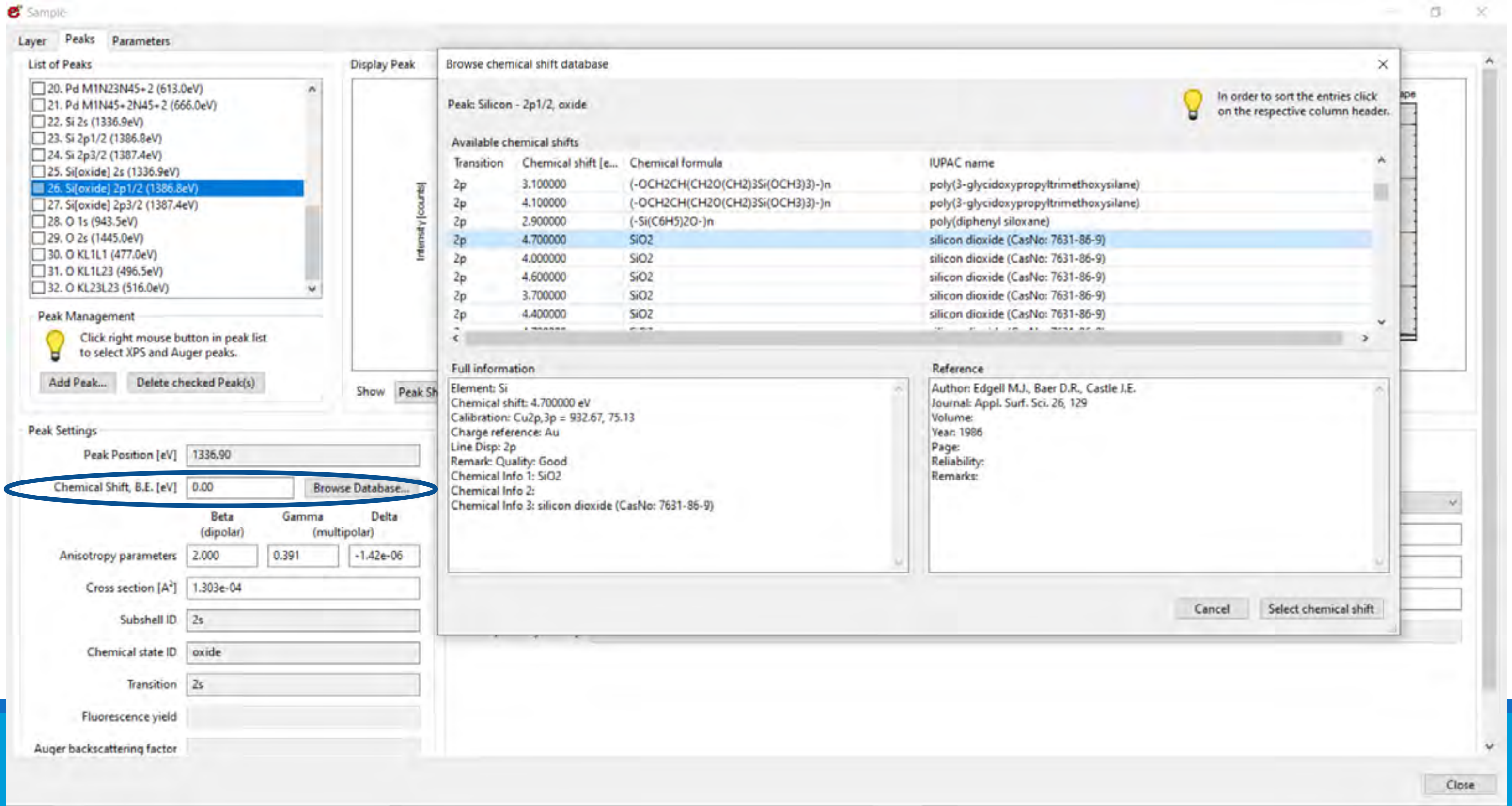


Image taken from [WebElements Periodic Table » Periodicity » Electronegativity (Pauling) » Periodic table gallery]

X-ray Photoelectron Spectroscopy

SESSA Exercise5: Chemical Shift

- Go to the Peaks tab and under Si 2p peaks click on the Chemical Shift and choose a Good estimation peak for the O bonded Si.

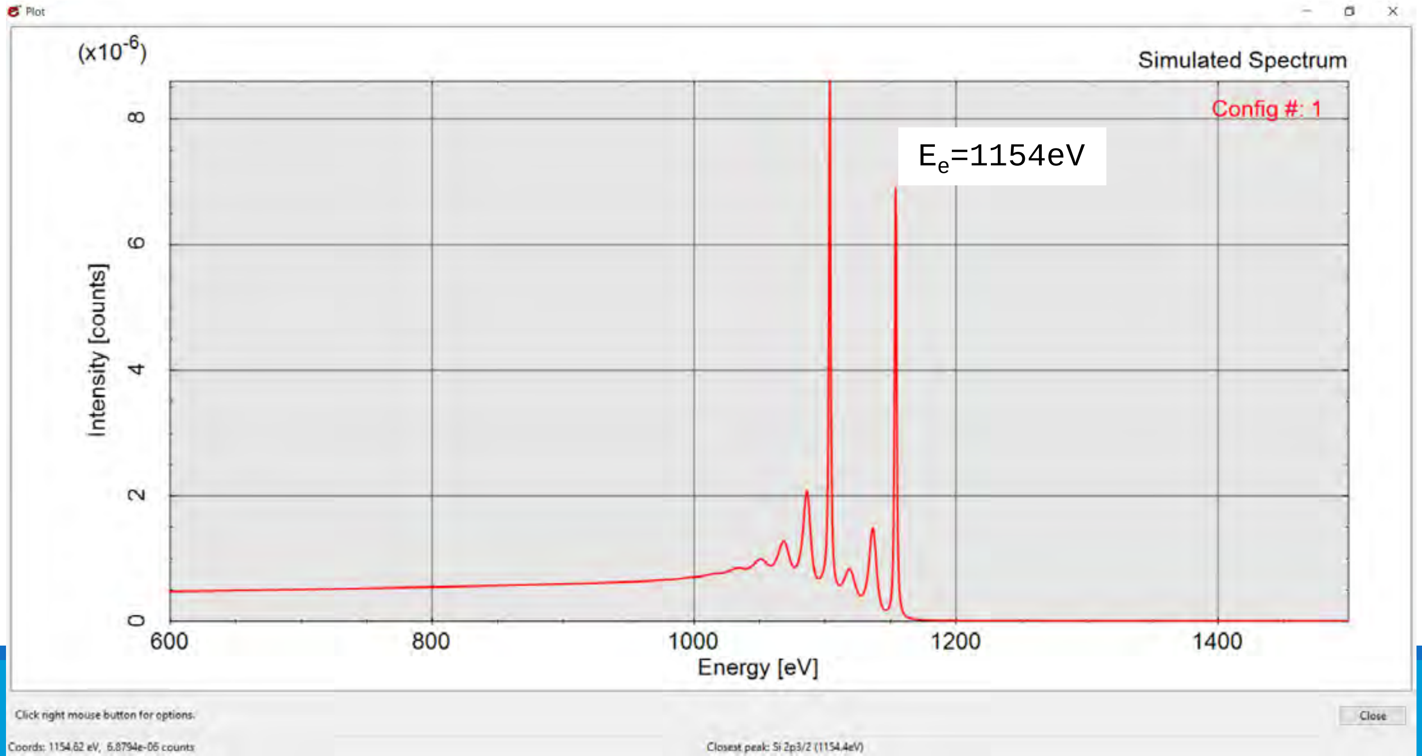


X-ray Photoelectron Spectroscopy

SESSA Exercise5: Chemical Shift

- Notice that 2p states are very close to each other for Si and yield a seemingly single peak.

Bare Si

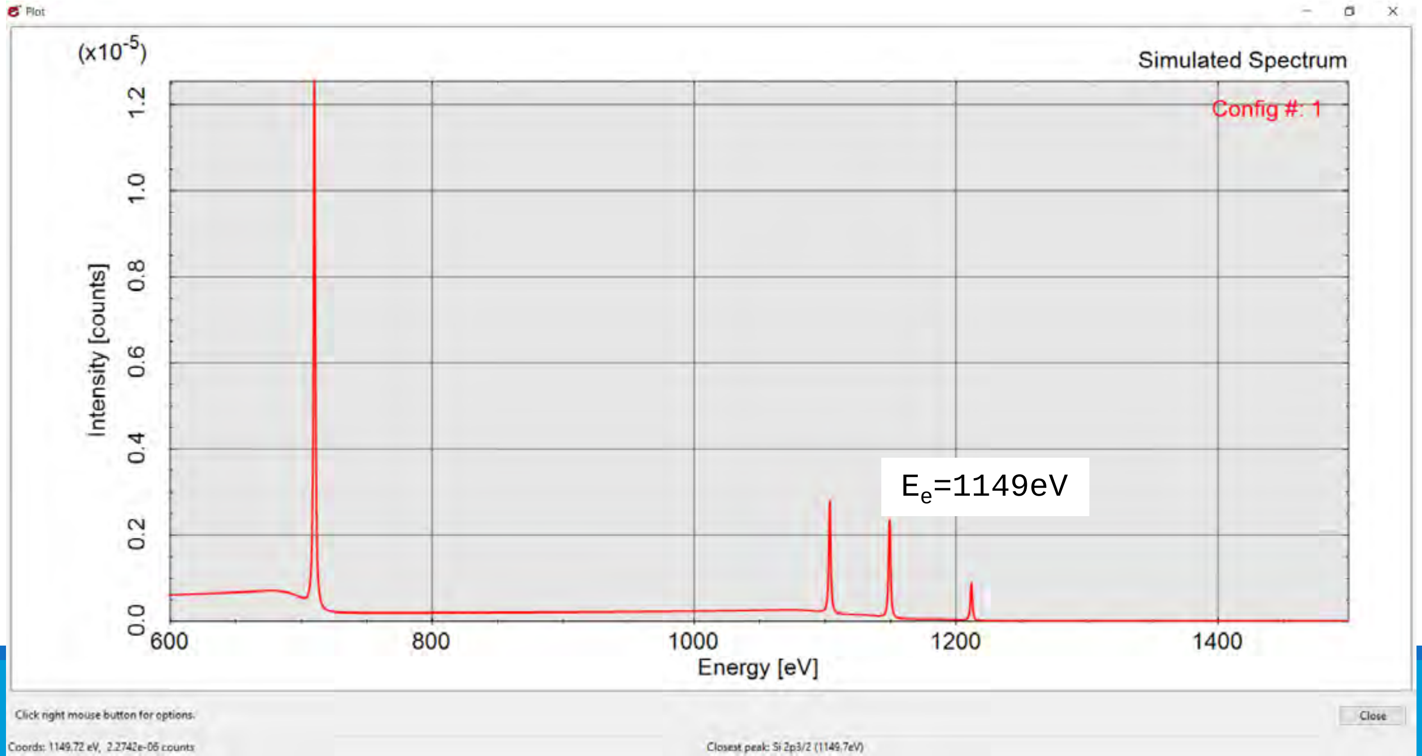


X-ray Photoelectron Spectroscopy

SESSA Exercise5: **Chemical Shift**

- Notice that 2p states are shifted by around 5eV to lower values, meaning that E_B is increased as a result of the O bond to the Si.

Oxidized Si



X-ray Diffraction

What is it and Why is it important?

- A very frequently used tool in order to determine
  - Crystal structure
  - Crystal size
  - Internal stress
  - Composition
- Elastic scattering (Bragg diffraction) of the X-rays from the examined materials are collected. Reflected X-rays will interfere and possess information about the crystallography.

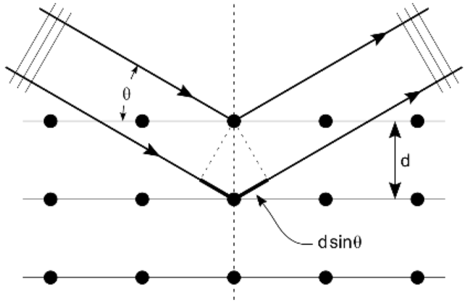


Image taken from Wikipedia

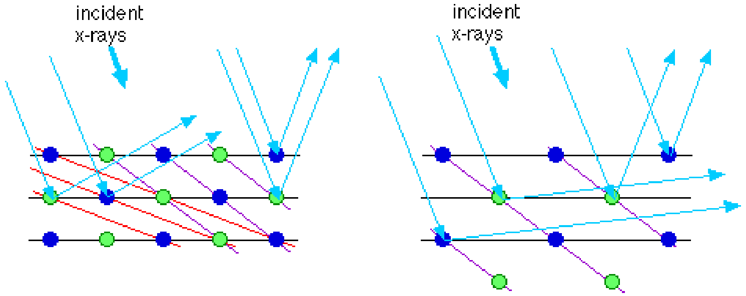


Image taken from Limits of resolution; X-ray diffraction (bu.edu)

X-ray Diffraction

Examining Interference from two sources separated by a distance

- Phet University of Colorado Boulder offers excellent illustrative tools to explain how the local positioning of the light sources can have an effect on the collected far-field diffraction patterns on a screen. This example can be linked to the reflection from the periodic atomic configurations: crystals. Wave Interference (colorado.edu)

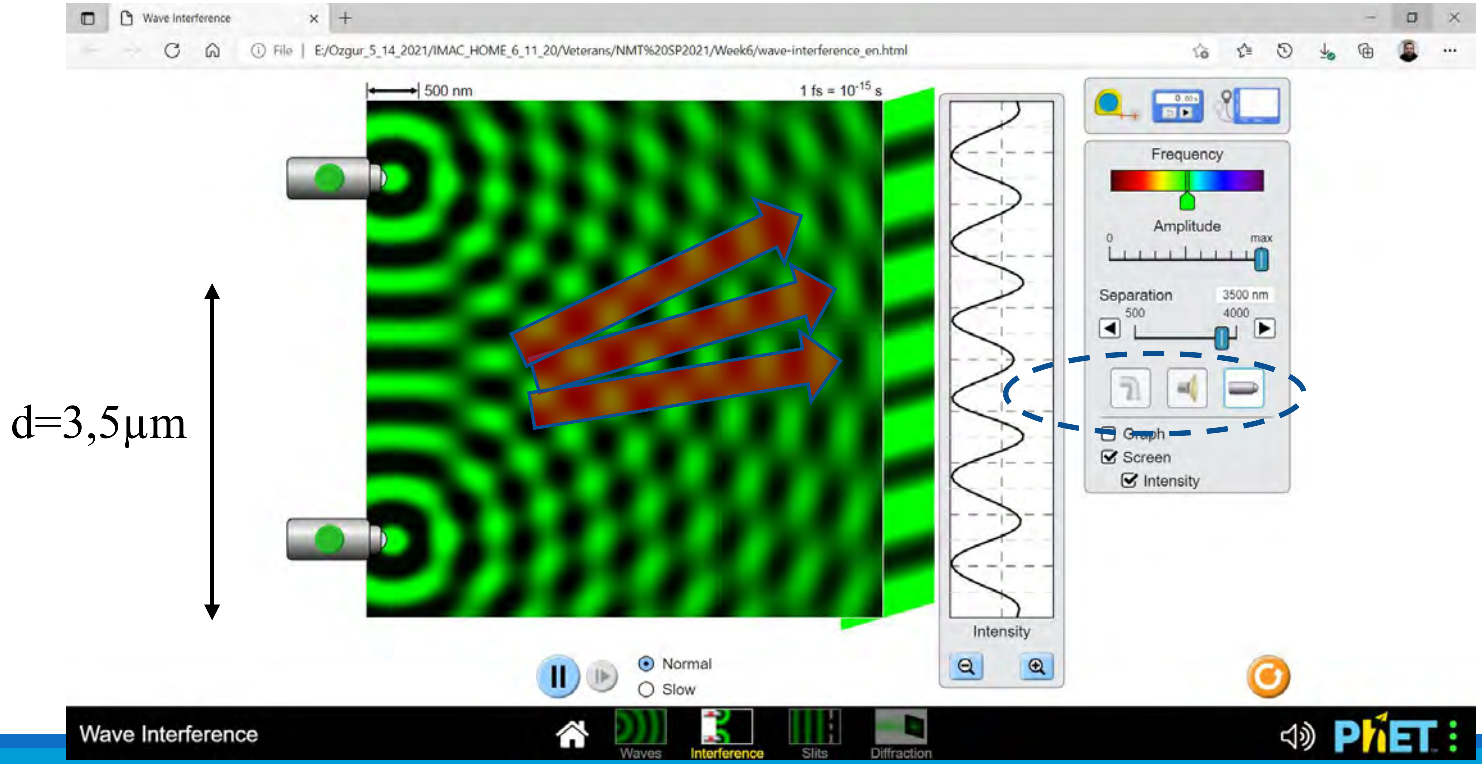
PhET INTERACTIVE SIMULATIONS

University of Colorado Boulder

X-ray Diffraction

Examining Interference from two sources separated by a distance

- Two sources separated by 3,5µm yields interference patterns that survive waves in the shown propagation directions (arrows).

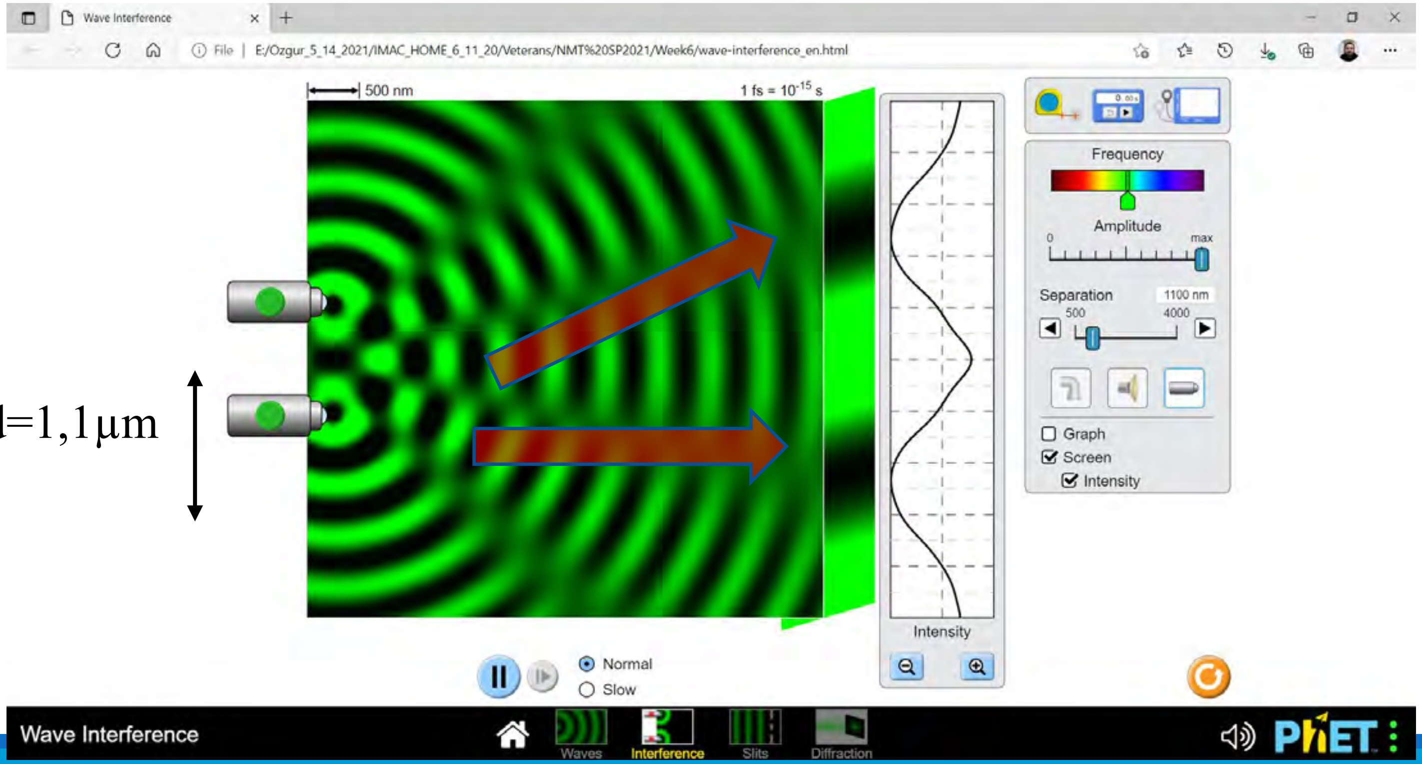


X-ray Diffraction

Examining Interference from two sources separated by a distance

- Two sources separated by 1.1 μm yields the given intensity profile on the screen.

d=1,1μm



X-ray Diffraction

Examining Interference from two sources separated by a distance

- Students can deduce that d and arrow directions, which constitute the diffraction pattern are related to each other. As d increases, the arrows make a larger angle (θ) wrt the horizontal axis. Accordingly:

$$\mathbf{d \propto \theta^{-1}}\ \textbf{(inversely proportional to each other)}$$

- Similarly, the reflections from planes of arranged atoms scattering rays 1-3 in the figure below can also be thought of the same form. The collection angle (θ) is related to the separation between these planes.

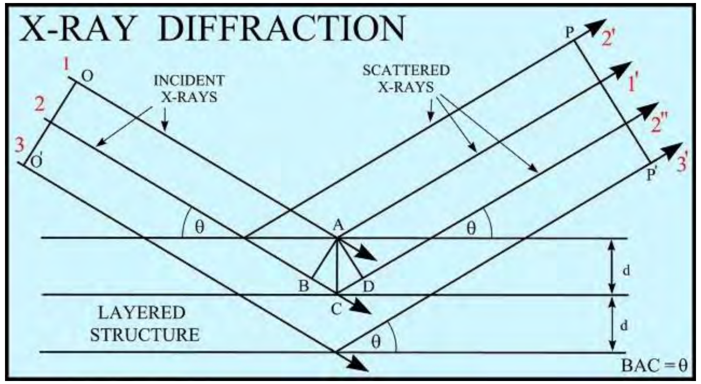
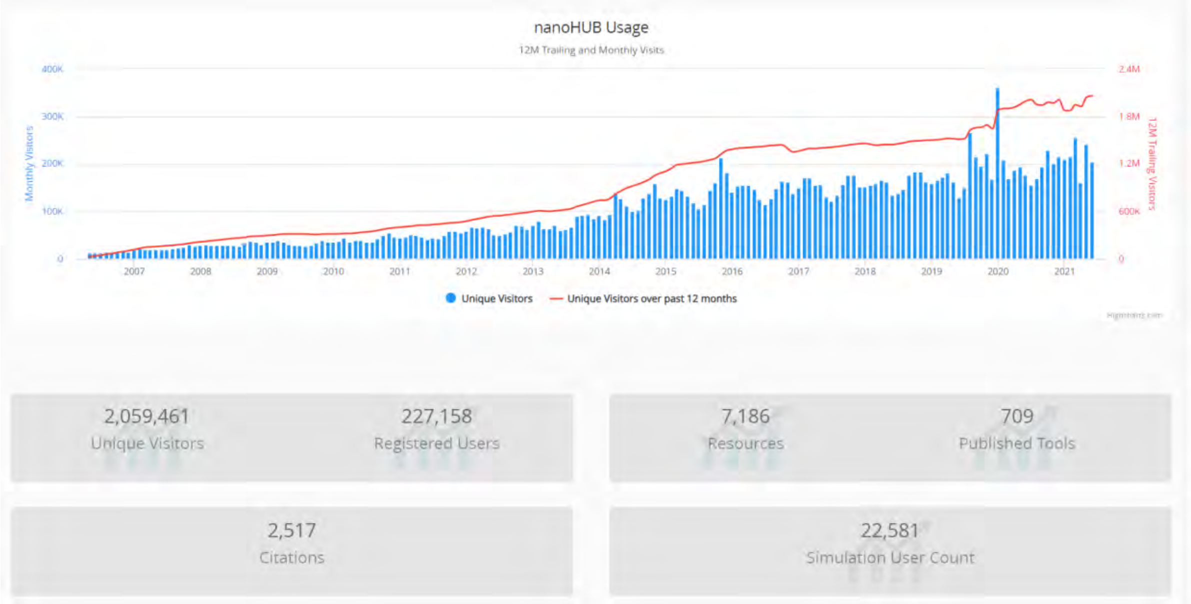


Image taken from [Bragg Diffraction | PhysicsOpenLab]

X-ray Diffraction

Examining Interference from two sources separated by a distance

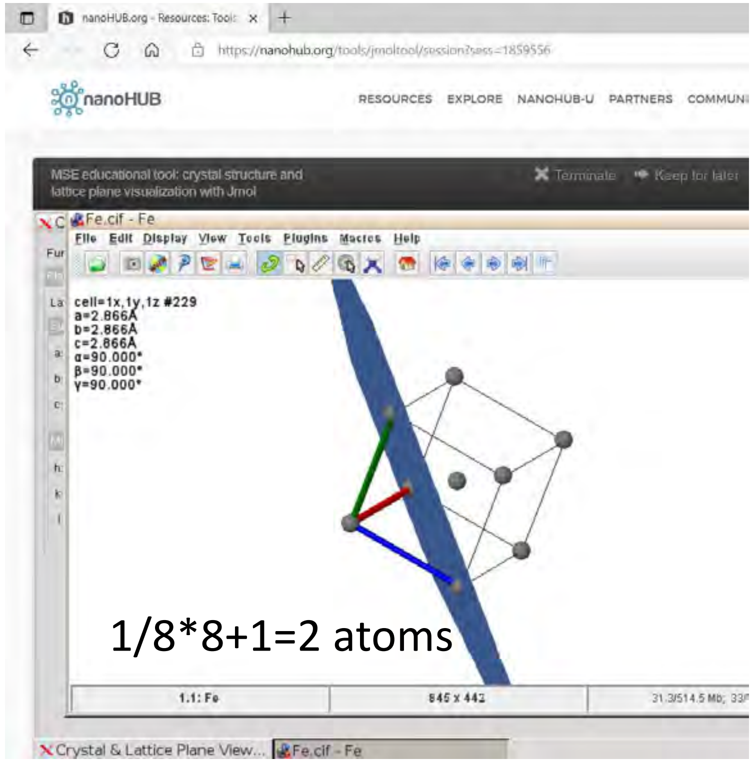
- Nanohub offers nanoHUB.org - Resources: MSE educational tool: crystal structure and lattice plane visualization with Jmol that helps easy visualization of the crystal planes and Bravais lattices.



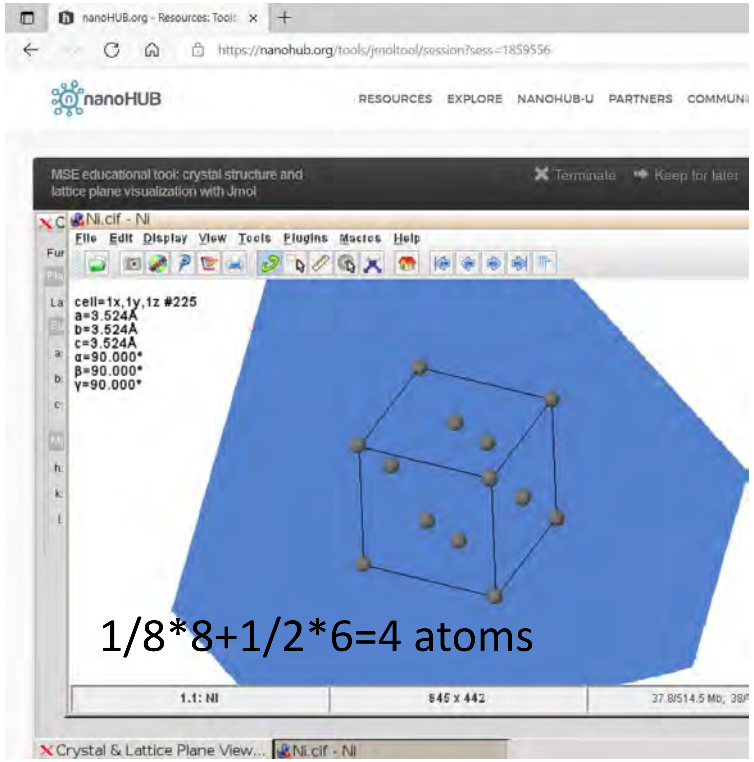
X-ray Diffraction

JMOL Exercise1: Counting number of atoms in BCC and FCC unit lattices.

BCC



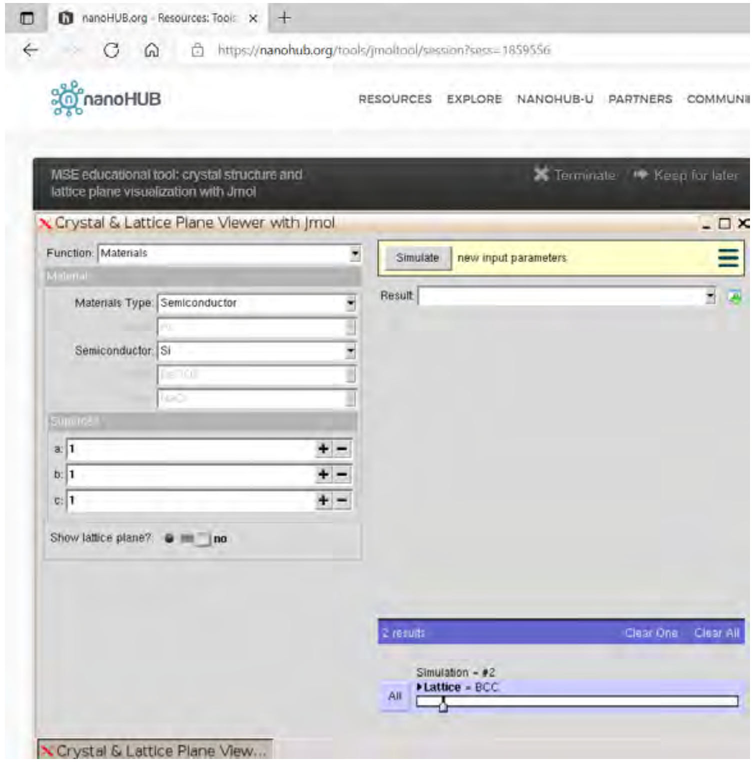
FCC

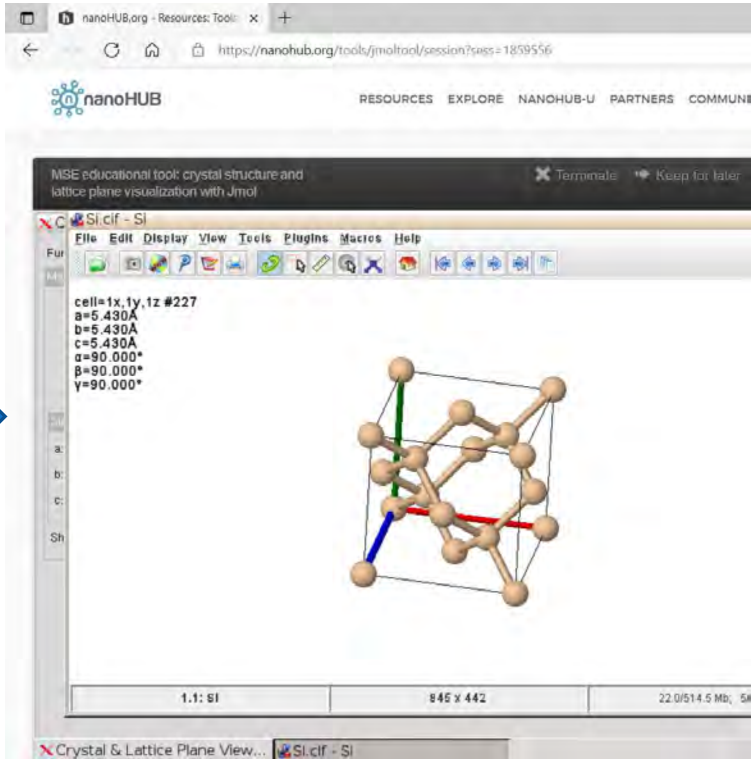


X-ray Diffraction

JMOL Exercise2: Si crystal structure and shortest distance between atoms.

Diamond lattice

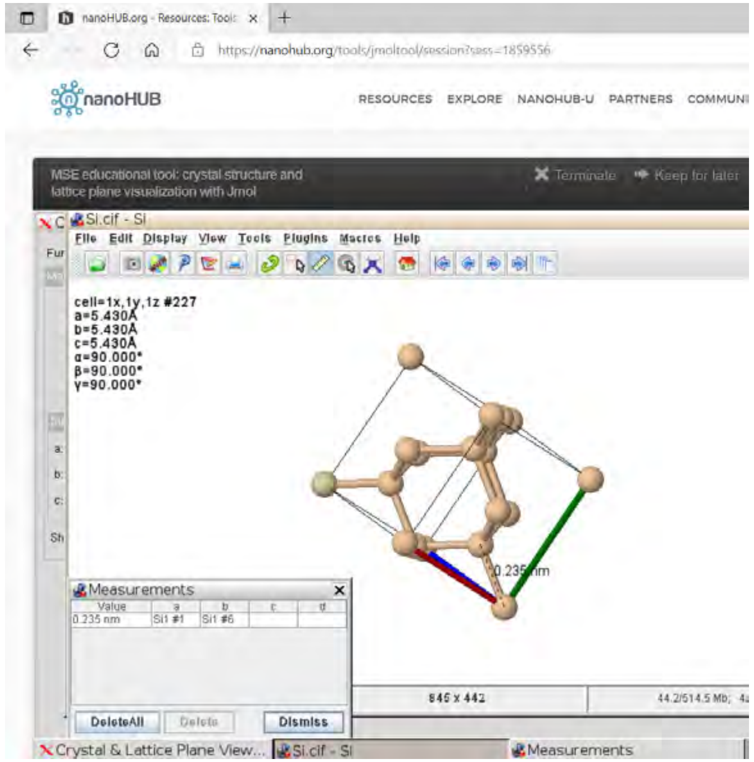




X-ray Diffraction

JMOL Exercise3: Si crystal structure and shortest distance between atoms.

Shortest Distance: 0.235nm

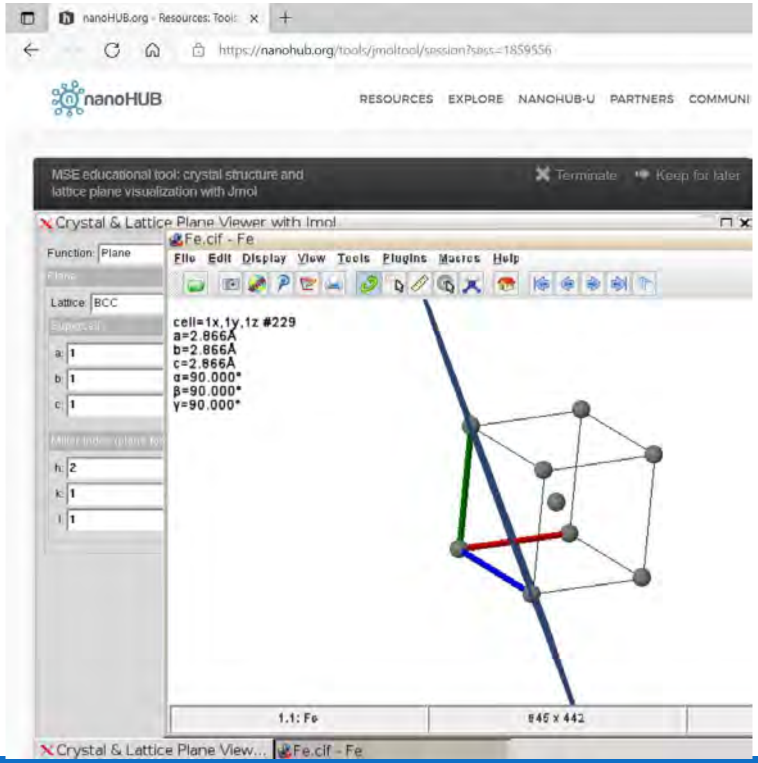


X-ray Diffraction

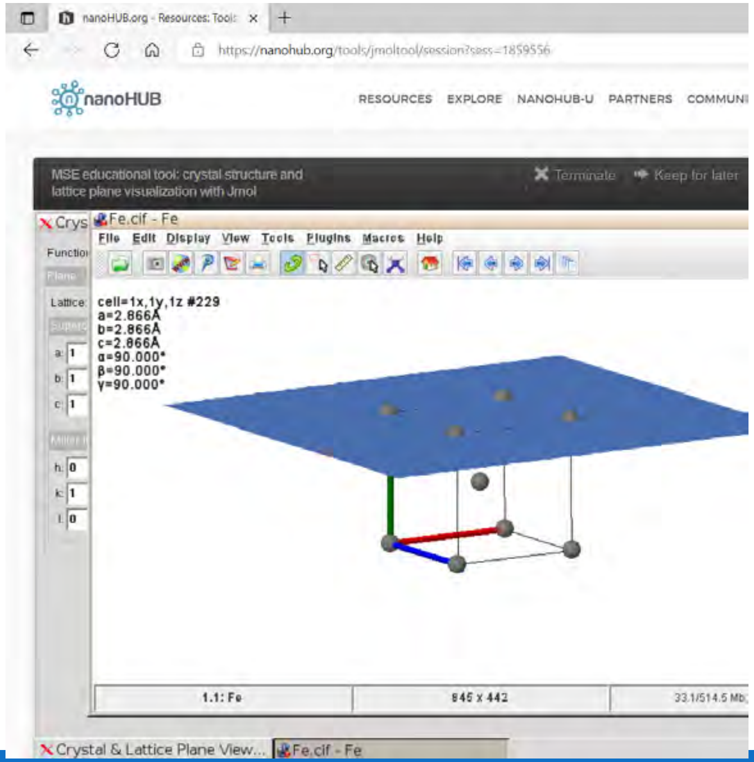
JMOL Exercise4: **Draw Miller planes for**

- (211) and (010) planes on BCC lattice.

(211)



(010)



X-ray Diffraction

XRD simulations:

- A typical configuration is shown below with the x-ray source on the left-hand side and the detector on the right-hand side. Optical elements are used to control the beam divergence.

Image taken from Wikipedia

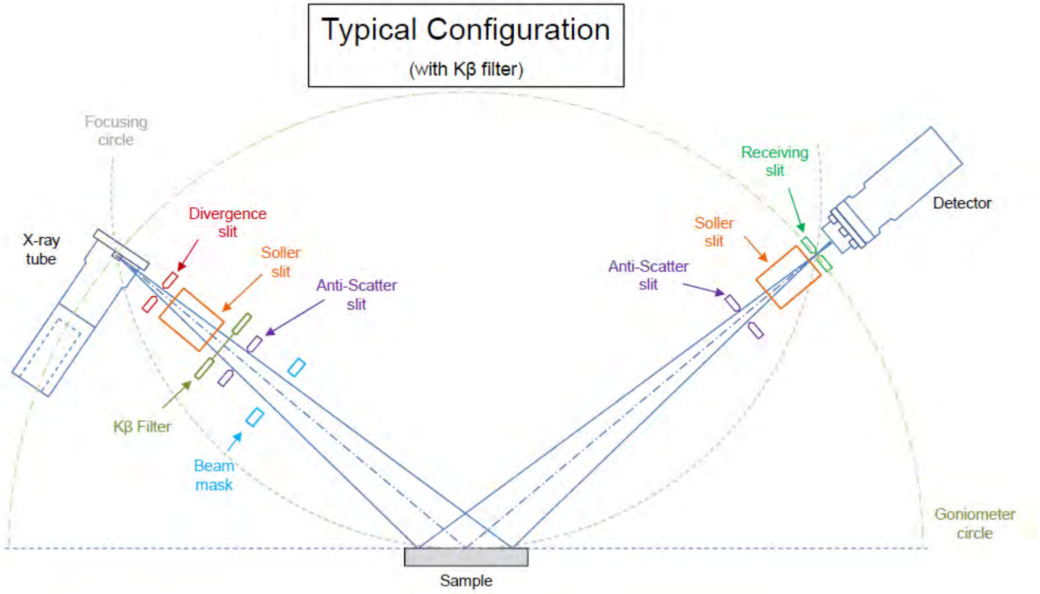
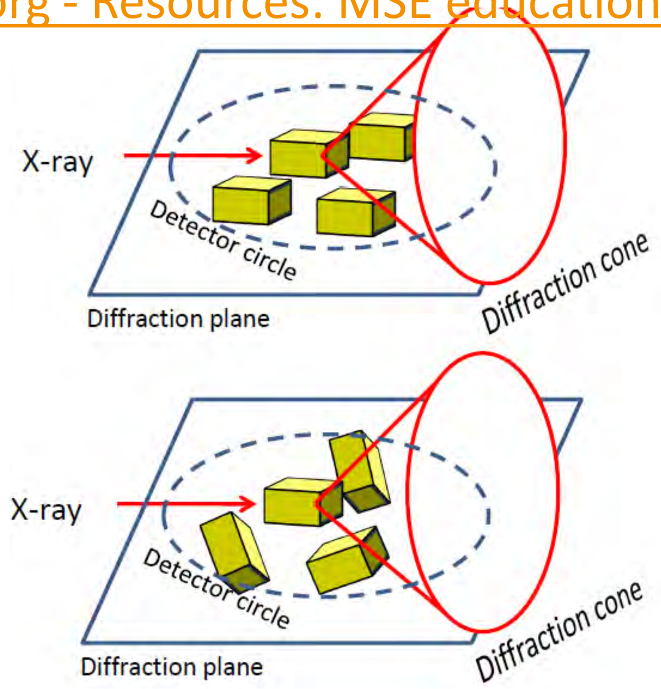


Image taken from RMS Foundation XRD Lecture Notes

X-ray Diffraction

XRD simulations:

- Students get convinced that the planes of reflections will create different diffraction cones at the exit side. Crystalline structures will generate point inside the diffraction cone. nanoHUB.org - Resources: MSE educational tool: X-ray diffraction (XRD) pattern



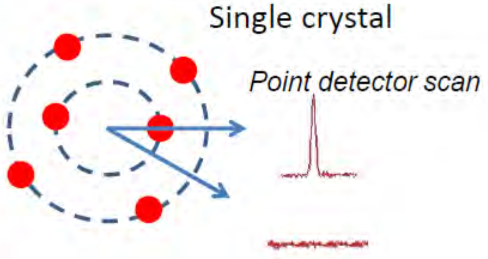
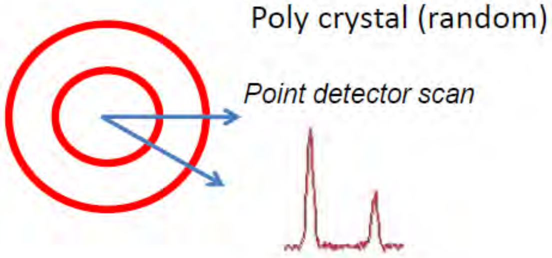
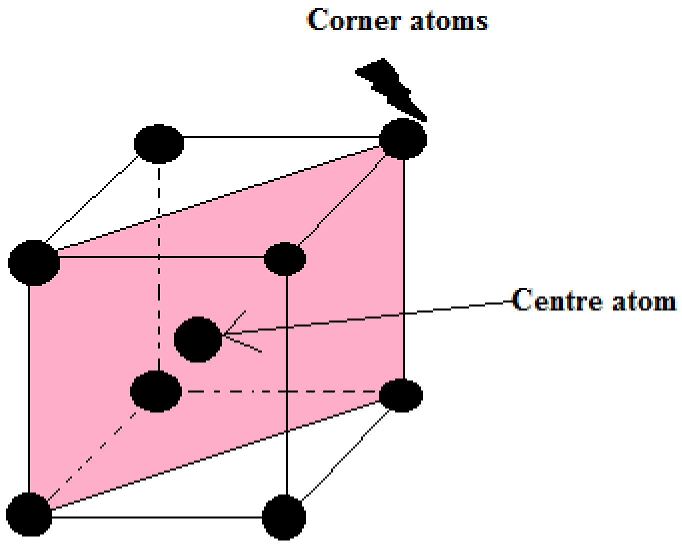


Image taken from Mauro Serdala's XRD lecture notes



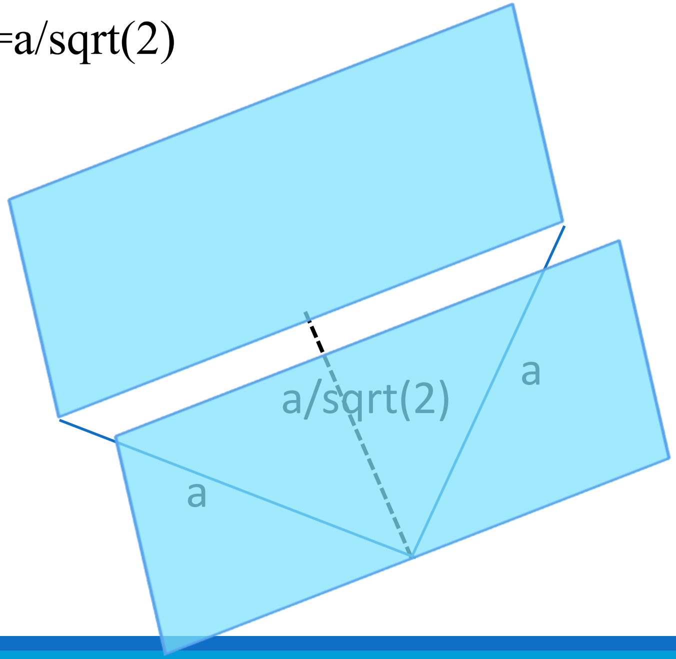
X-ray Diffraction

XRD Exercise1: Collect peak locations for BCC and verify for (110) plane.



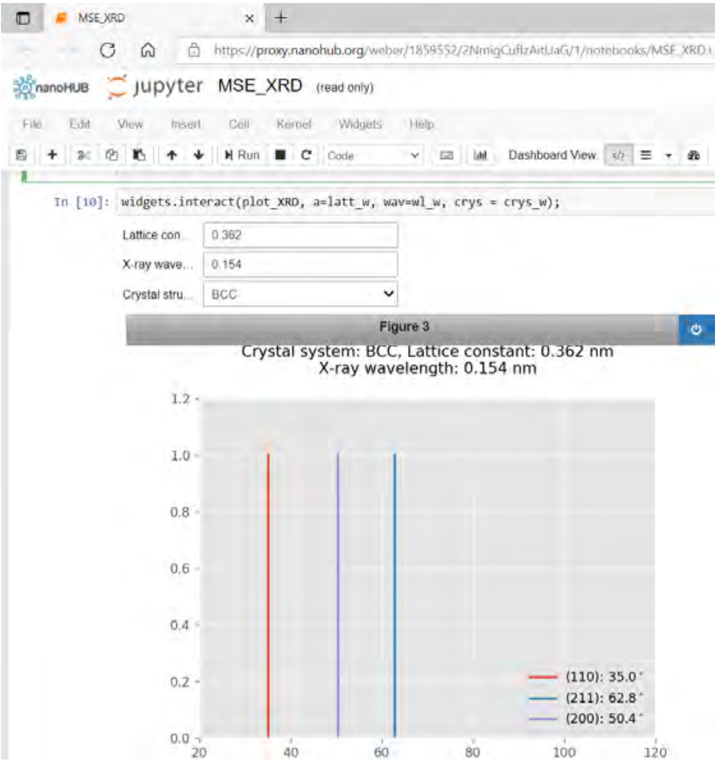
(100) plane

These reflection planes are separated by a distance d of:
d=a/sqrt(2)



X-ray Diffraction

XRD Exercise1: Collect peak locations for BCC and verify for (110) plane.



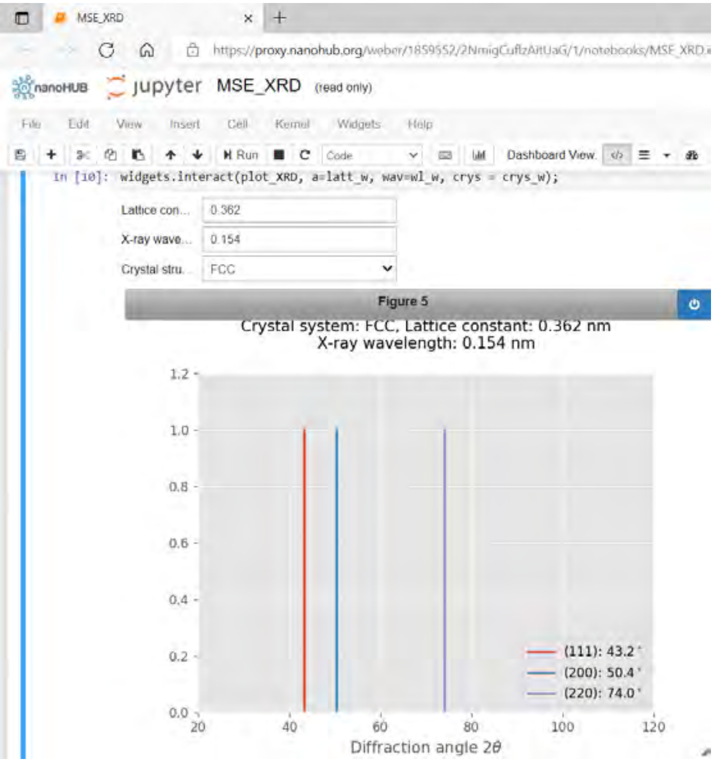
$$2d\sin\theta = n\lambda$$

According to Bragg formula:
n=1, λ=0.154nm (CuKα), d=a/sqrt(2), a=0.362nm

θ=sin^{-1}(0.154/(2*0.362/sqrt(2)))=17.5 degrees

X-ray Diffraction

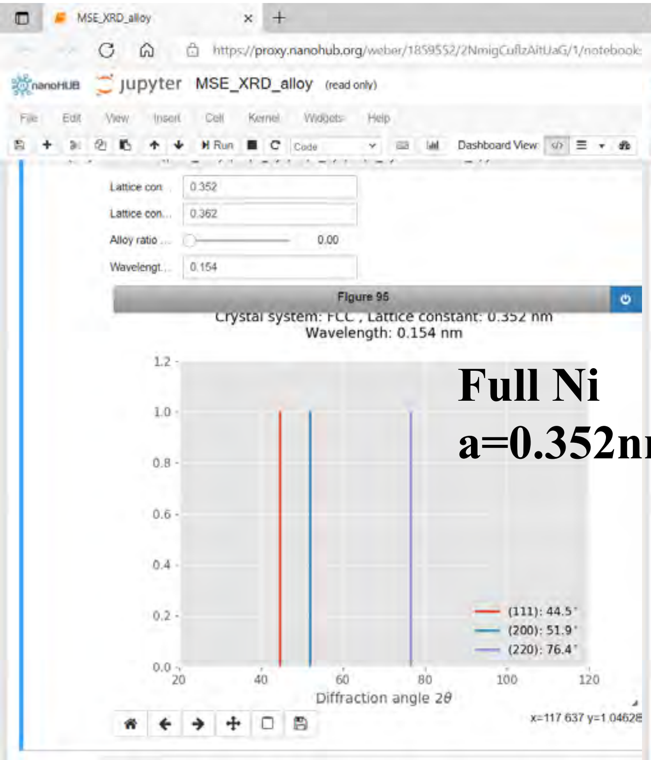
XRD Exercise2: Collect peak locations for FCC

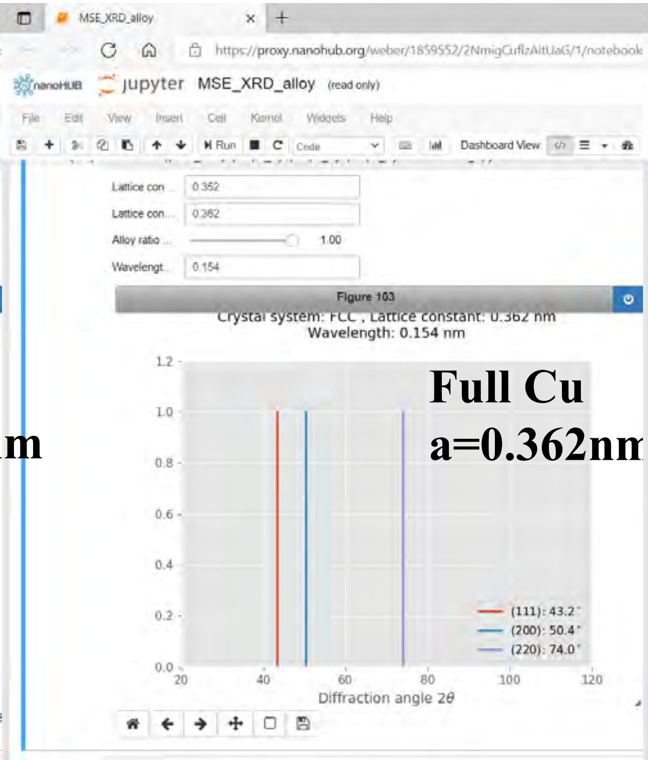


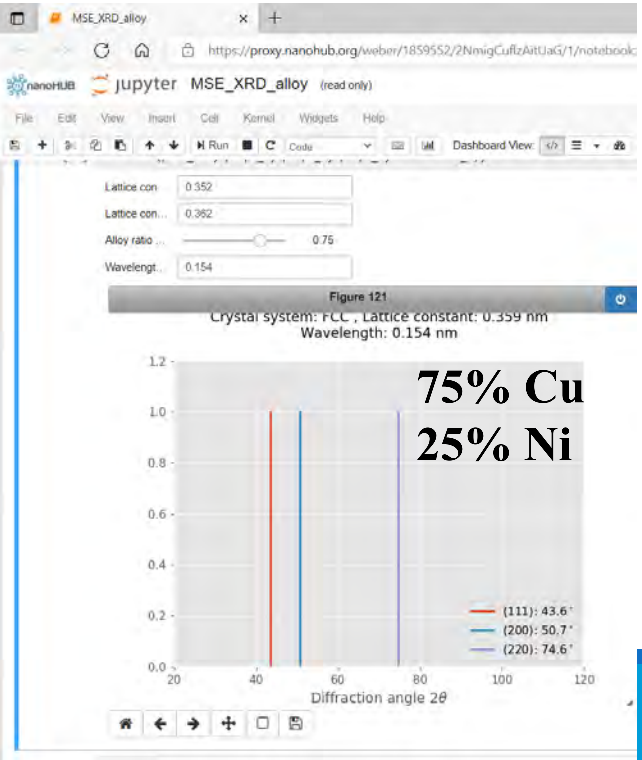
X-ray Diffraction

XRD Exercise3: Finding alloy ratio of Ni-Cu alloy

- Instructor comes up with a hidden alloy ratio and asks students to figure it out by intelligent trials remembering that d and θ are inversely proportional to each other. Let us say (220) plane 2θ=74.6.



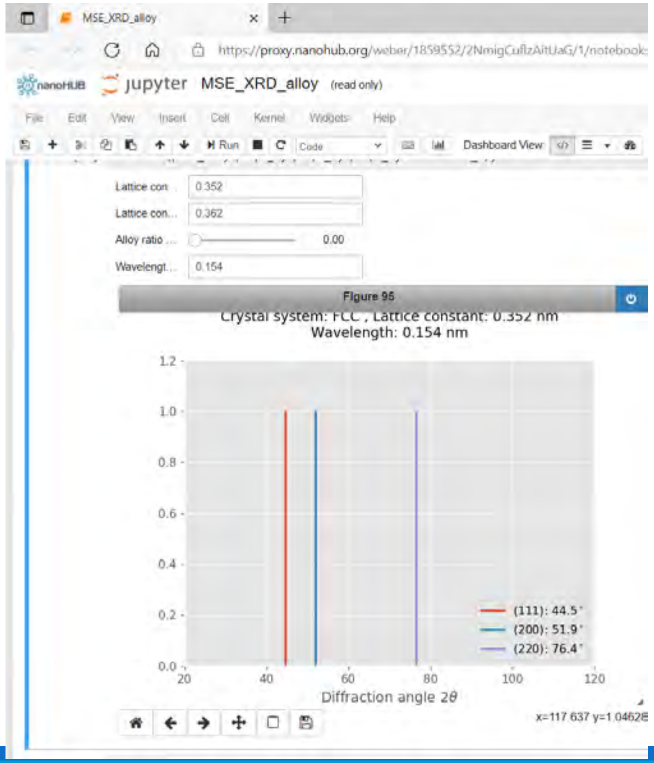


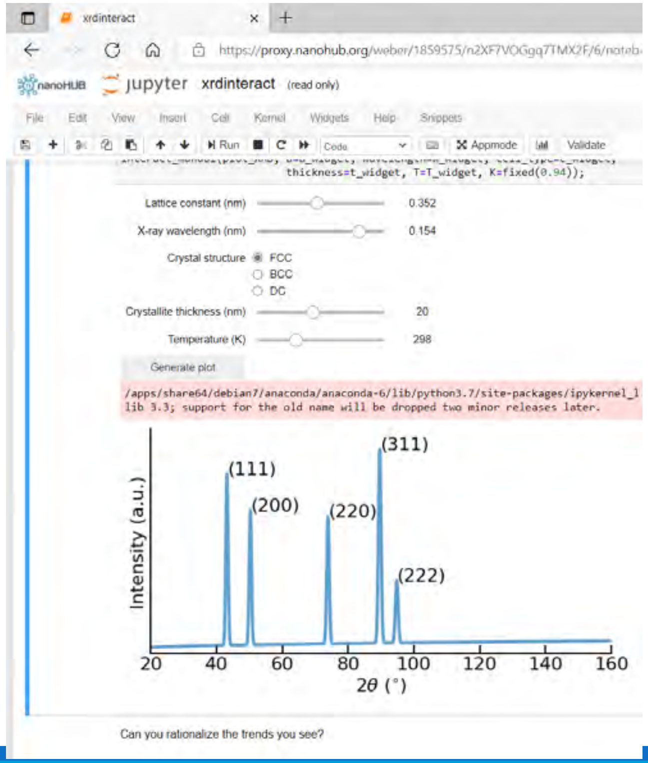


X-ray Diffraction

[nanoHUB.org - Resources: XRD interactive trends plot]

- XRD interactive trends enables a simple calculation of the more realistic peaks with valid amplitudes





X-ray Diffraction

nanoHUB.org - Resources: XRD interactive trends plot

- XRD interactive trends enables a simple calculation of the more realistic peaks with valid amplitudes. Sherrer's equation is also integrated to take into account the grain sizes (thickness parameter)

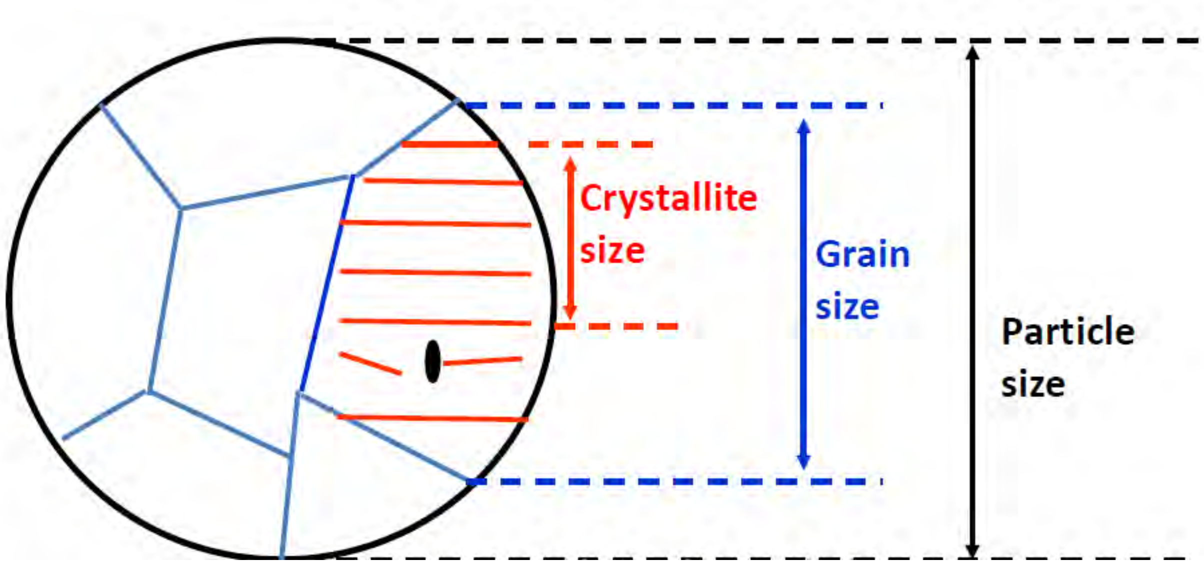


Image taken from Mauro Serdala's XRD lecture notes

X-ray Diffraction

XRD Exercise4: Comparing the grain size effects on FWHM

- Grain size determines the peak broadening

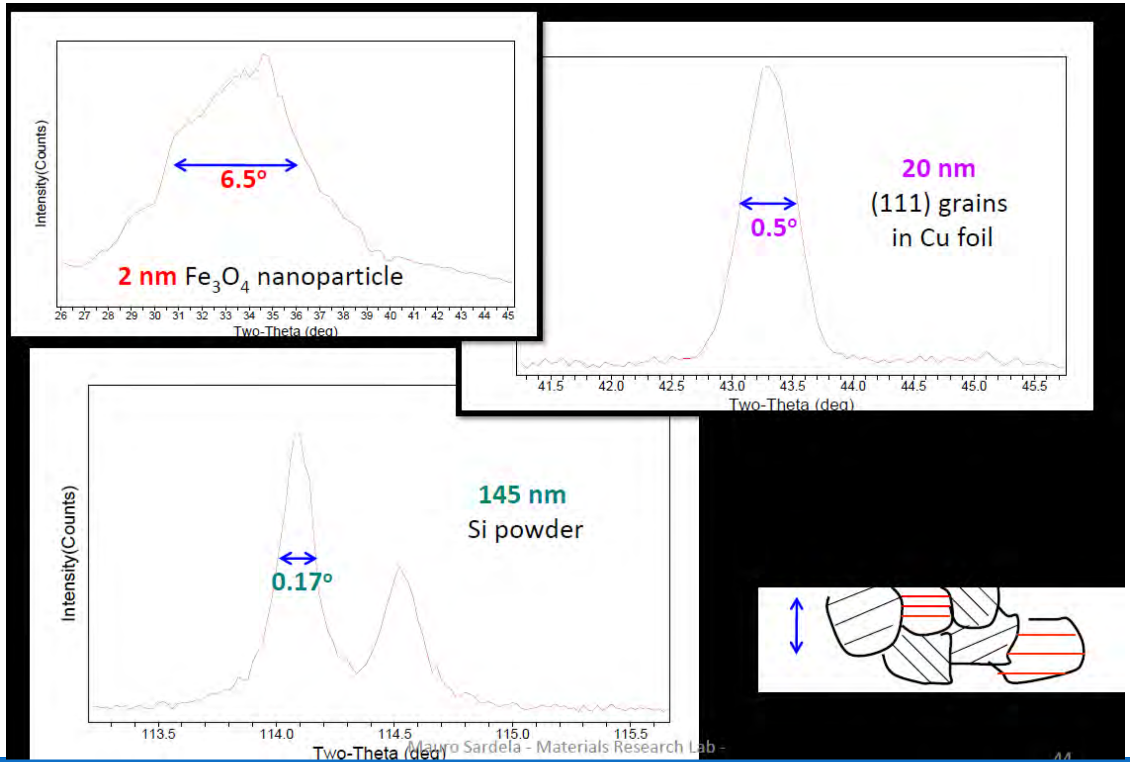
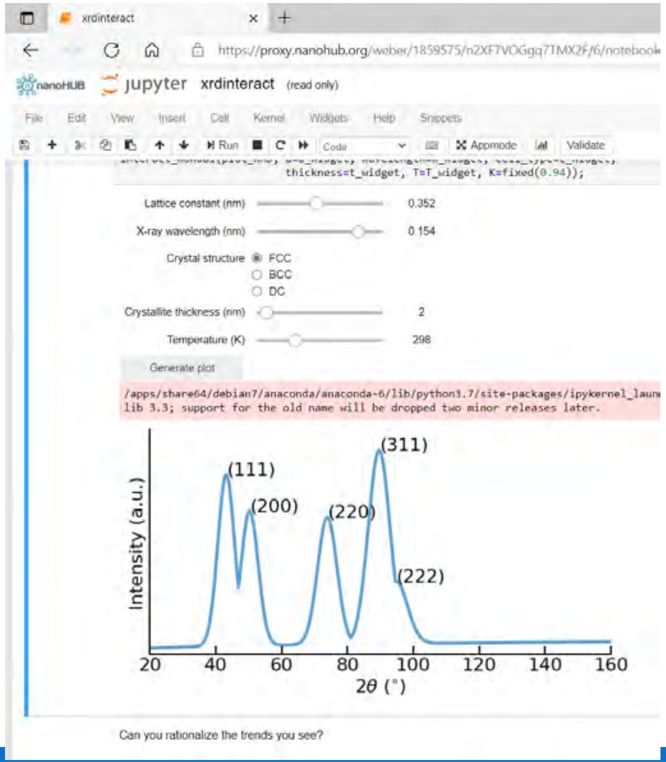


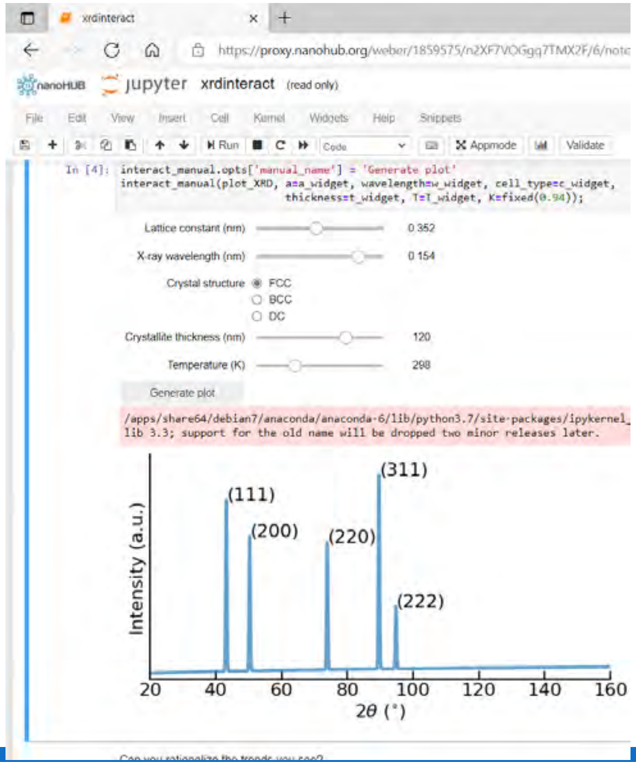
Image taken from Mauro Serdala's XRD lecture notes

X-ray Diffraction

XRD Exercise4: Comparing the grain size effects on FWHM

- Students observe the changes when grain size is entered as 2nm and 120nm





Student Reception and Applicability

- All these tools have been employed in Spring/Summer Capstone nanotechnology (intro level) courses in 2020 and 2021 by Center for Nanotechnology Education and Utilization (CNEU) at Penn State.
- The best adaptability of the simulation tools are for nanotechnology programs that can be offered at associate/undergraduate/grad level. On the other hand, they can be employed as a lab exercise for 200-grad level Chemistry/Physics courses.
- The tools offer a great wealth of understanding for the students on tool operation and capabilities. Two main questions have been assessed:
  - What is XPS/XRD used for?
  - How does it work?

Student Reception and Applicability

The tools have received much attention and interest from the students as they facilitate a **problem-centric learning experience utilizing computational methods**. The main outcomes can be summarized as:

- As in the case of XRD tool on nanohub, interested students also **get exposed to python** (a scripting language) which is commonly used today.
- Instead of the traditional pedagogical approaches, which are based on traditional unidirectional material transfer from the instructor to the students, participants can focus on **real life problems**.
- Students can work in **small teams to focus on case studies** by altering nanocharacterization parameters, which are linked to fundamental sciences.
- The instructor is **relieved from the restrictions of having thousands of dollar worth tools** ready for the class demonstrations.
- The simulation tools offer the **ideal remote teaching environment** under Covid-19 restrictions.
- The simulations also **cut down the idle pump-down and other related waiting times, sample preparation process** of the tools. However, it has to be emphasized that all of those steps are invaluable hands-on exposure opportunities for the students and the simulation tools cannot completely replace what they can offer.

First time use tips for instructors

Phet Simulations are very straight-forward, designed primarily for high school students. They are very easily adaptable for a higher-level discussion as shown in the previous slides. The instructor might need to install Java for some Apps: How do I install Java ? Web-based simulations are more encouraged in order to prevent the extra hurdle for compatibility issues.

SESSA instructions are carefully shared in the document step by step. Installation requires a few additional steps as the students need to fill in a form for approval. Instructors are advised to assign the installation part as a HW for the students to save time.

Nanohub simulations require the users to get an account. Instructors are advised to assign this as a HW for the students, as well.

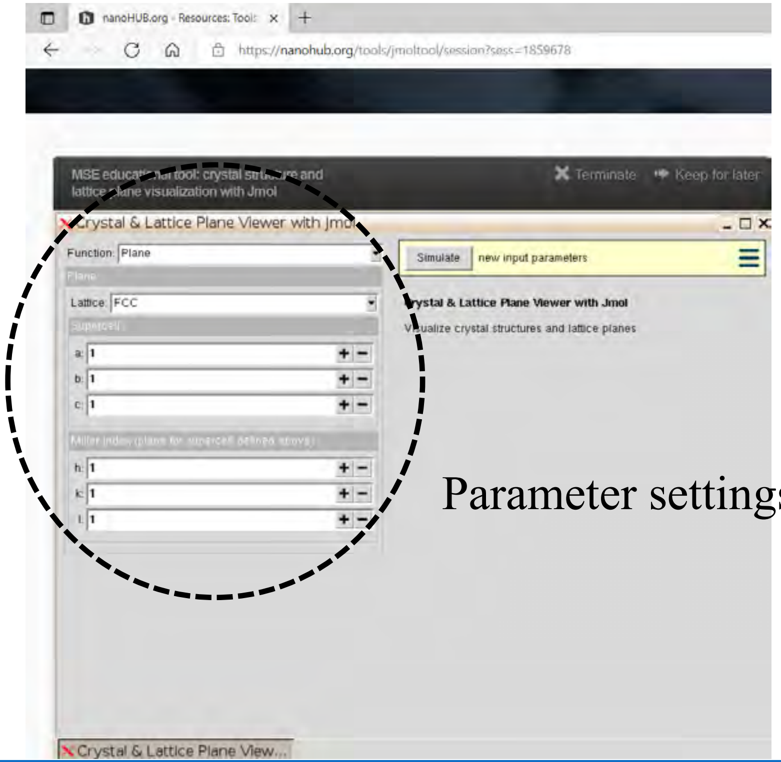
First time use tips for instructors

NanoHub simulations **do not necessitate a strict requirement** on the computational resources on students' side, individually. All tools are run online on their servers, which has been recognized as a great advantage.

CAUTION and Limitation: Nanohub and Phet simulation tools are designed to educate the essentials of the X-ray tools and may not offer a completely correct physical picture! The exercises and values obtained should be treated accordingly for instructional purposes. For example, XRD inteactive nanohub tool does not calculate the peak intensities obtained from different planes. SESSA, on the other hand, is a well received research level tool developed by respectable researchers in the field and offered by NIST. The instructor will find an incredible depth of discussion here: Simulation of Electron Spectra for Surface Analysis (SESSA)Version 2.2 User's Guide | NIST It has to be reminded that many of these in-depth discussions might be outside of the scope for an undergraduate/associate degree program.

First time use tips for instructors

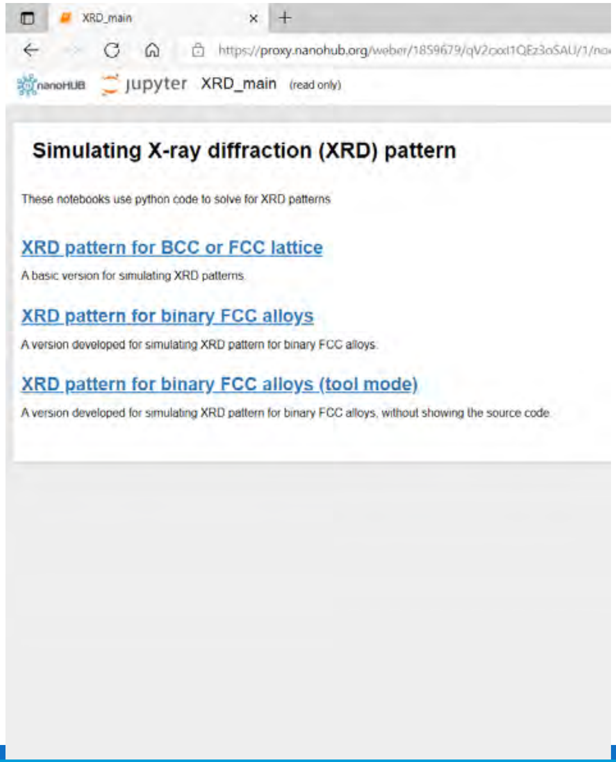
Nanohub JMol simulations: Instructors will have the chance to select the parameters to run once the simulations start. Instructors are advised to follow the given exercises by entering the same parameters for the first run. Additional documents are also offered by nanoHub for each simulation tool.



Parameter settings

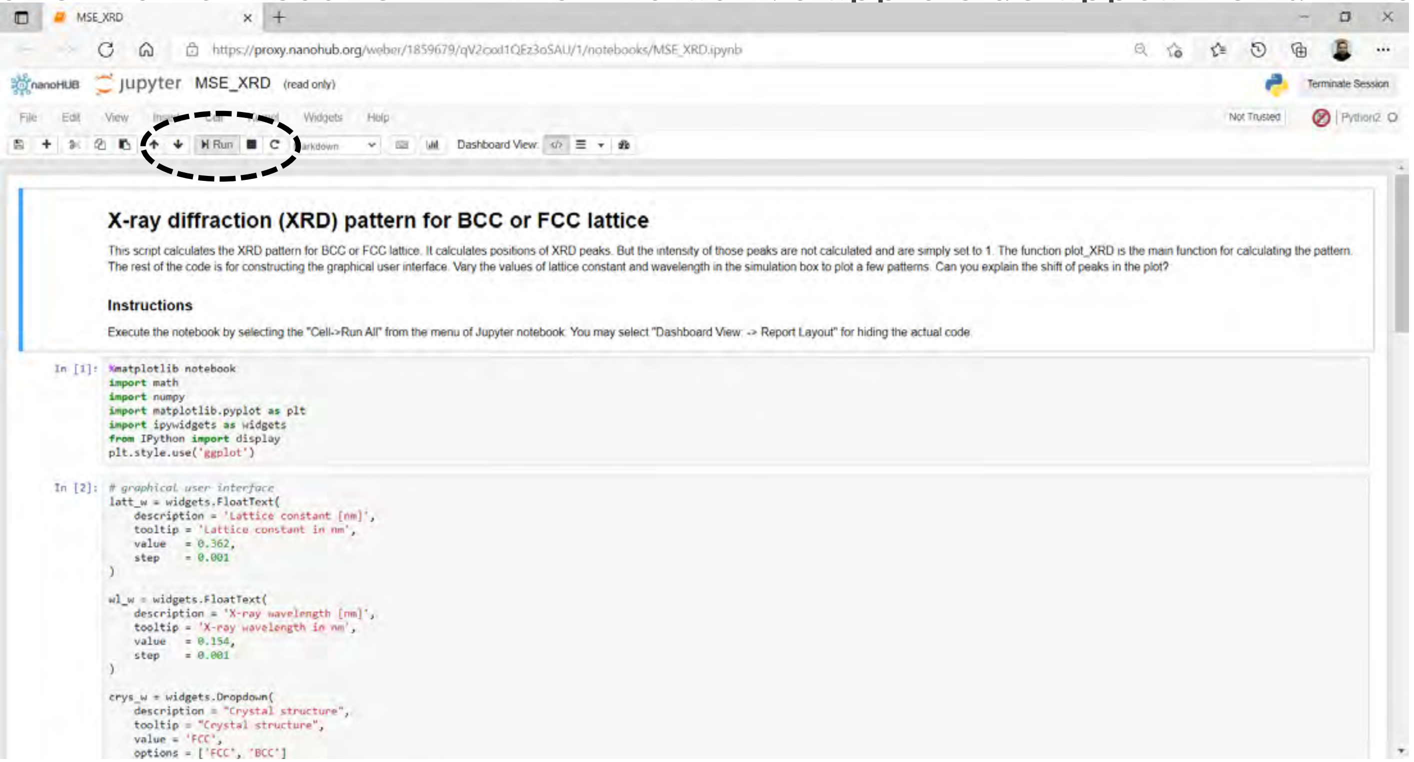
First time use tips for instructors

Nanohub Interactive XRD simulations: Once the instructor logins to the XRD tools, the following options will be available. Clicking on each link will take the instructor to one of the python based simulation environments.



First time use tips for instructors

Nanohub Interactive XRD simulations: Python exposure is not the priority but a definite plus for the interested students. The instructor can just skip the coding section by clicking on Run button to move to the next section till the interactive applets do appear to run the exercises.



Conclusion

1. **Online visualization and simulation tools help to enhance teaching/learning of nanoscale phenomena in Physics, Chemistry, Engineering, Engineering Technology, Material Science, Environmental Sciences, and Biological sciences.**
2. **Use of Visualization and Simulation promote students' interest in STEM education.**
3. **Increased interest in STEM education is expected to enable the students to join a rapidly growing workforce in the field of nanotechnology.**
4. **Free online RAIN facility is an excellent resource for introducing nanotechnology to the students at a small institution with limited funds.**
5. **RAIN allows to learn about nanotechnology instruments before acquiring them.**
6. **nanoHUB, based at Purdue University, is an excellent simulation platform for introducing and analyzing nanotechnology phenomena at all educational levels at no cost to the institutions.**
7. **Phet Interactive Simulations, based at University of Colorado, is an excellent resource for teaching Physics, Chemistry, Environmental Sciences, Material Science and Biological sciences in undergraduate programs.**
8. **Physicell is a robust, scalable code for simulating viral dynamics of SARS-CoV-2 (coronavirus/COVID-19) in a layer of epithelium and several submodels (such as single-cell response, pyroptosis death model, tissue-damage model, lymph node model and immune response).**
9. **Compucell3D is flexible modeling platform that allows rapid simulations for cancer, developmental biology, evolution, immune system, tissue engineering, toxicology, non-cellular soft material and viruses such as Covid-19.**

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Thanks for attending this presentation….Any Comments…Questions…Feedback? Please contact us via e-mail:

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To know what you know and what you do not know, that is true knowledge.
--- Confucius

The art of knowing is knowing what to ignore.
--- Rumi