Web-Based Simulation and Remote Access Visualization Tools for Engineering and Technology Curricula

July 31, 2024

Dr. Ahmed S. Khan

Fulbright Specialist Scholar

Ex. Dean of the College of Engineering & Information Sciences

DeVry University, Addison, IL

Dr. Atilla Ozgur Cakmak

Assistant Professor of Electrical Engineering

School of Engineering, Seymour and

Esther Padnos College of Engineering and Computing

Grand Valley State University

Allendale, MI

cakmaka@gvsu.edu

Dr. Sala Qazi

qazi@sunypoly.edu

In Memoriam

Dr. Sala Qazi

Emeritus Professor & Chair
School of Information Systems and Engineering Technology
State University of New York Institute of Technology (SUNYIT),
Utica, New York

Dr Sala (Salahuddin) Qazi was a Professor Emeritus at SUNY Poly. During his thirty-year tenure at SUNY Poly, he was chairman of the EET department, coordinator of the BS program in photonics, and Director of the MS program in advanced technology, which he helped to develop.

Dr Qazi authored numerous articles in the area of fiber doped amplifiers, wireless security, MEMS and photovoltaic energy. He also co-authored two books in the area of "Nanotechnology for Telecommunications" and "Solar Energy Systems and Technologies." After retiring, he authored a book on "Standalone Photovoltaic (PV) Systems for Disaster Relief and Remote Areas."

He was the recipient of several awards, including the William Goodell award for research creativity at SUNY Poly; he was recognized by the Mohawk Valley Engineering Executive Committee for engineering professionalism; and he forged closer relations with the IEEE Mohawk Valley section. He was a CO-PI for a conference on "High Capacity Optical Networking and Enabling Technology, [HONET]". Dr. Qazi was a life member of IEEE and ASEE.

Atilla Ozgur Cakmak
Assistant Professor of Electrical Engineering
School of Engineering, Seymour and Esther Padnos
College of Engineering and Computing
Grand Valley State University, Michigan

Atilla Ozgur Cakmak graduated from Sabanci University, Istanbul, Turkey with a BSc degree in Microelectronics Engineering in 2003. He obtained his MSc degree in Computer Science and Electronics Engineering also from Sabanci University in 2005.
Dr. Cakmak earned his PhD degree from Bilkent University, Ankara, Turkey in 2012 from the Department of Electrical and Electronics Engineering. After a brief postdoctoral experience at Bilkent University within NANOTAM (Nanotechnology Research Center),.
Dr. Cakmak joined Penn State in 2013 as a postdoctoral researcher to work on thin film solar cells. Dr. Cakmak got promoted to Assistant Teaching Professor at Penn State within the Department of Engineering Science and Mechanics in 2018. He offered graduate and undergraduate level courses in the field of nanotechnology and nanofabrication.
Dr. Cakmak is now an Assistant Professor of Electrical Engineering in School of Engineering in Grand Valley State University, Michigan. Dr. Cakmak co-authored more than 20 papers in the leading journals in his expertise field of nanophotonics and microwave engineering.
Dr. Cakmak also contributed with educational publications to the field of nanotechnology and nanoscience. He is an editor of Journal of Advanced Technological Education and a guest editor of MDPI. He has also been contributing as a reviewer to various optics/photonics, applied physics and nanotechnology themed journals.

Dr. Ahmed S. Khan

Professor of Electrical Engineering
Fulbright Specialist Scholar
Ex. Dean of the College of Engineering & Information Sciences
DeVry University, Addison, Illinois

Dr. Khan has more than forty years of progressively responsible experience in instruction (online and onsite), applied research, curriculum development, program and institutional accreditation, management, and supervision of academic programs at DeVry University. Dr. Khan held many academic positions that include Senior Processor, Chair, and Dean of the College of Engineering & Information, DeVry University, Addison, Illinois, USA. Dr. Khan also served as the National Curriculum Manager at the national headquarters of DeVry University, where he supervised and managed curriculum development and implementation of BSEEt & MSEE programs at 25 DeVry campuses located in the United States and Canada. Dr. Khan received an MSEE from Michigan Technological University, an MBA from Keller Graduate School of Management, and his Ph.D. from Colorado State University. His research interests are in the areas of Nanotechnology, New Teaching & Learning Techniques, and Social and Ethical Implications of Technology. He is the author of many educational papers and presentations. He has authored/coauthored many technical books, including the Science, Technology & Society (STS) series of books that include *Technology and Society: Issues for the 21st Century & Beyond* (used globally in the academic programs of more than 200 universities), *and Nanotechnology: Ethical and Social Implications, to* stimulate, inspire, and provoke awareness of technology's impact on society. Dr. Khan is a senior member of the Institute of Electrical and Electronics Engineering (IEEE), and a member of American Society of Engineering Education (ASEE). Dr. Khan has also served as program evaluator for the accreditation agency ABET.

Web-Based Simulation and Remote Access Visualization Tools for Engineering and Technology Curricula

Simulation and visualization tools promote students' understanding of phenomena at nanoscale.

This session will focus on application of web-based simulation tools and remote access visualization (RAIN, Nanohub, Physicell, Phet, Compucell3D) for teaching, research, and collaboration in the areas of nanotechnology, material science, environmental science, electrical engineering, biological sciences, physics, chemistry, photonics, and other areas.

Educators can use these web-based tools to enhance students' learning of complex concepts at nanoscale without acquiring expensive equipment.

Simulation experiences at GVSU for photovoltaic applications will also be presented.

Web-Based Simulation and Remote Access Visualization Tools for Engineering and Technology Curricula

Web-Based 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.**

Web-Based Simulation and Remote Access Visualization Tools for Engineering and Technology Curricula

Order of Presentation

- Online Simulation and Visualization Tools
  - NanoHub
    - Examples of simulations using nanoHub
    - Phet Interactive Simulations
    - Physicell
  - CompuCell3D
    - Examples of Simulation of Covid-19 Virus
  - RAIN: Remote Accessible Instruments for Nanotechnology
  - MYSCOPE: SEM & TEM

- Use of Online Simulation Tools (SEM & TEM) at GVSU

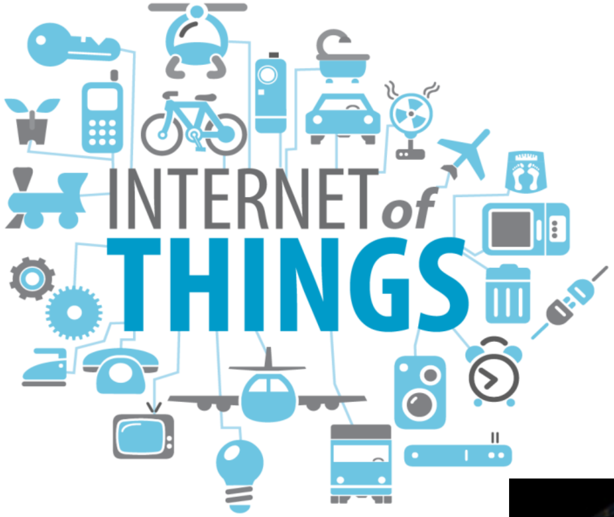
Conclusion

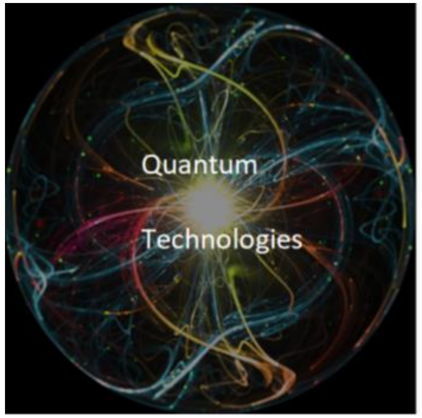
Web-Based Simulation and Remote Access Visualization Tools for Engineering and Technology Curricula

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*.

Emerging Technologies





Emerging 4IR Technologies

Nanotechnology, Robotics and Artificial Intelligence (AI)

Web-Based Simulation and Remote Access Visualization Tools for Engineering and Technology Curricula

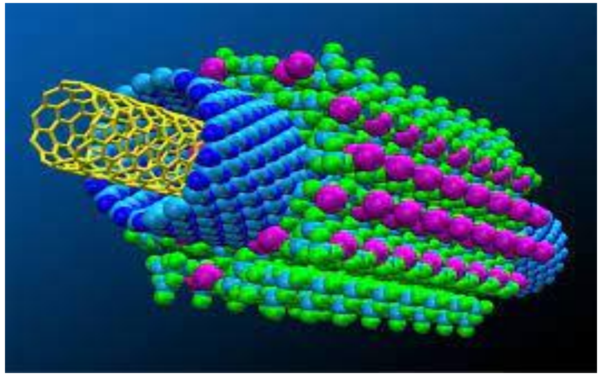
Key Challenges

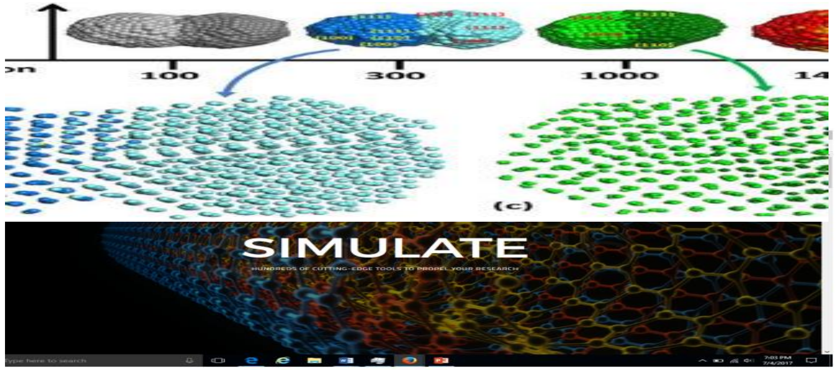
- Teaching, Learning and Research in new and emerging technologies require state of the art laboratories equipped with expensive equipment and associated support facilities.

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

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

Learning through Visualization and Simulation at the Nanoscale





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,

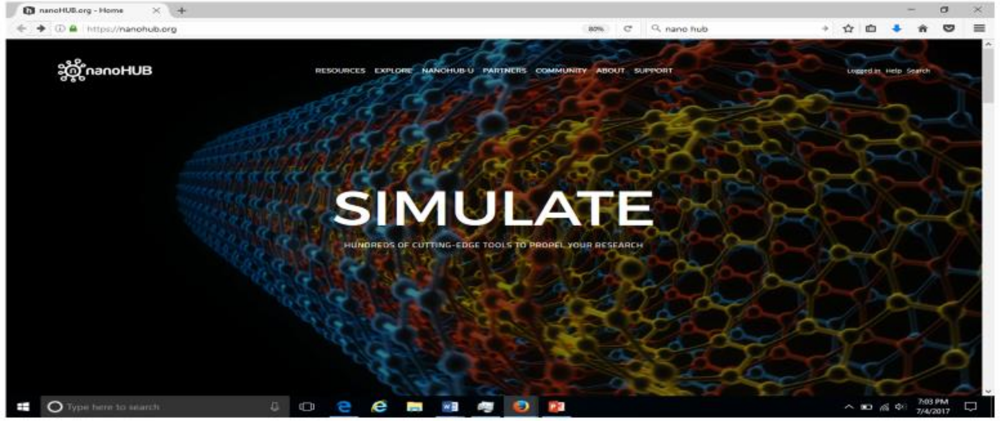
and (d) enhancing the presentation of “dry” concepts by integrating theory and practice

Learning through Visualization and Simulation at the Nanoscale

Nanohub.org

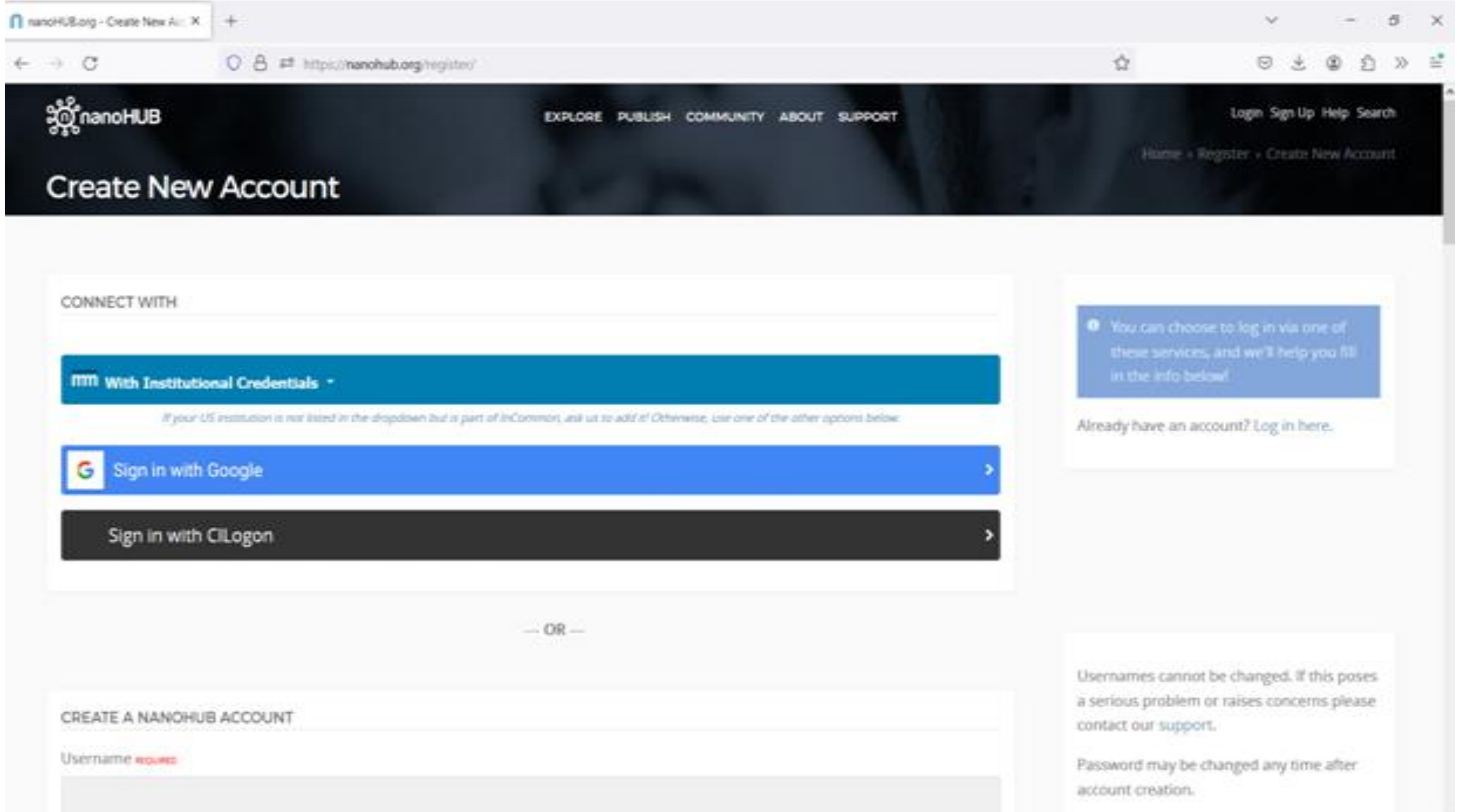
- Computing Cloud located at Purdue University
- 500+ simulation tools & apps
- 1.4 million users Worldwide
- 6500 resources

Crystal Viewer Tool
Nanohub.org



Learning through Visualization and Simulation at the Nanoscale

Nanohub.org....Creating a User Account

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Tools
Most Popular
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Surface Chemistry
Pharmaceutical Formulations
Polymeric Materials
Consumer Packaged Goods

Model & Simulate

Rapid Education and Research

500+ Apps for Everyone

READY-TO-USE, INTERACTIVE, SELF-CONTAINED

- Nanoelectronics (Map View)
- Materials
- Photonics
- Most Popular

MORE

Tools for Development

ASSEMBLE YOUR OWN COMPONENTS

- Jupyter
- Linux workstation
- UQ
- Machine Learning
- Rappture I/O and GUI building

MORE

Tools for Experts

CONFIGURE & CUSTOMIZE SIMULATIONS

- Materials
- Electronics
- nanoBIO
- Nano Manufacturing

MORE

Engines / Frameworks

COMPUTATIONAL SCIENCE COMPONENTS

- Materials (MD, ab-initio, ...)
- Electronics
- Photonics

MORE

Develop Software

Assemble your own components

Developer Kits

ASSEMBLE YOUR OWN RESEARCH FLOW

- Jupyter Notebooks
- Linux workstation
- Rappture I/O and GUI building

Workflows

GO BEYOND A SINGLE SIMULATION

- Uncertainty Quantification
- Machine Learning
- Pegasus Docs & Example

Engines / Frameworks

COMPUTATIONAL SCIENCE COMPONENTS

- Materials (MD, ab-initio, ...)
- Electronics
- Photonics

MORE

Documentation

NANOHUB/HUBZERO SOFTWARE STACK

- Tool Development Workshop
- Rappture BootCamp 2014
- Rappture Docs
- Tool Developers (submit, paths etc)

MORE

Share & Publish

Join 2,000+ Contributors

Why / Impact

BUILD REPUTATION AND HELP OTHERS

- Web-of-Science & Google Scholar Citations
- Notable Quotes

Apps, Tools, & Data

R&D FOR YOU AND ENABLE OTHERS

- How to Overview
- Start a Tool Publication

Video Lectures / Courses

TEACH OTHERS

- Best Practices
- How To: Advanced Video Editing for nanoHUB
- Submit Video Here

Teaching Materials

TEACHING MATERIALS

- Submit Text Documents
- Submit Animations

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Sign up for their online courses

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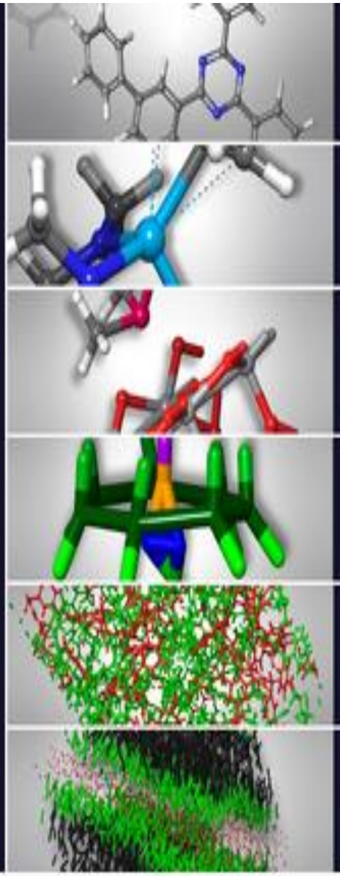

- Organic Electronics
- Homogeneous Catalysis
- Surface Chemistry
- Pharmaceutical Formulations
- Polymeric Materials
- Consumer Packaged Goods

Overview Solutions Use Cases Learn Download

MATERIALS SCIENCE

Online certification courses

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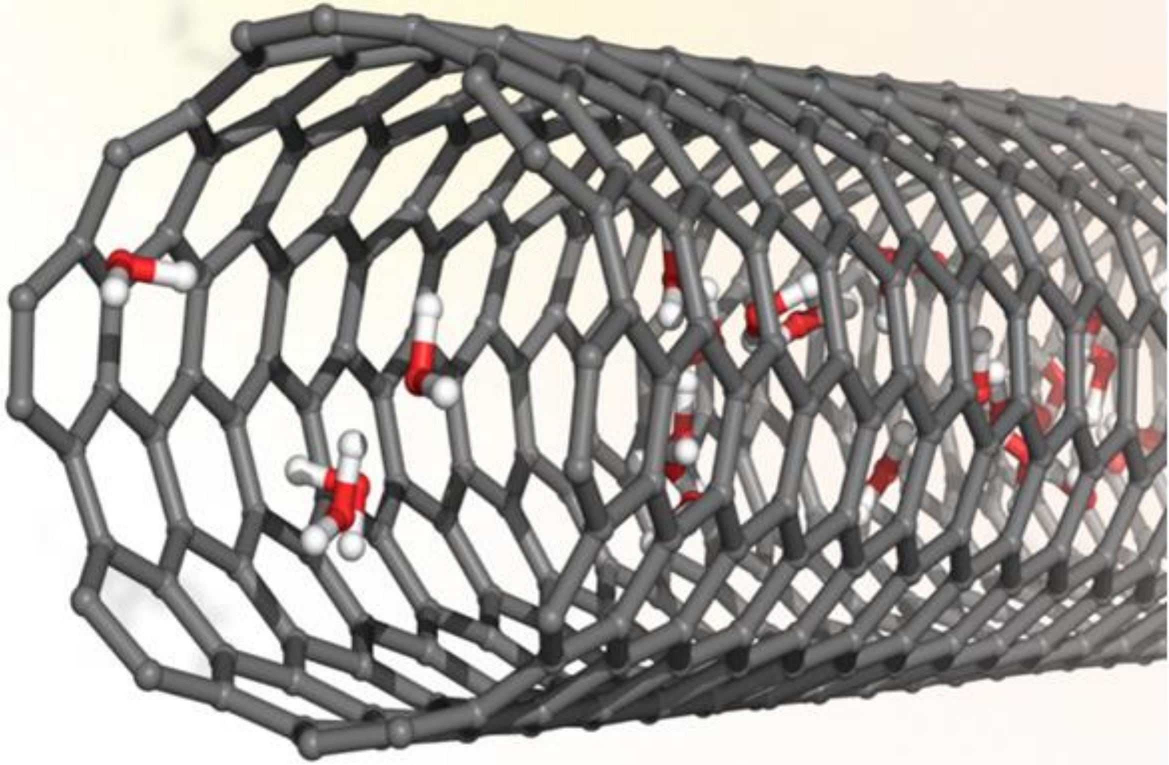
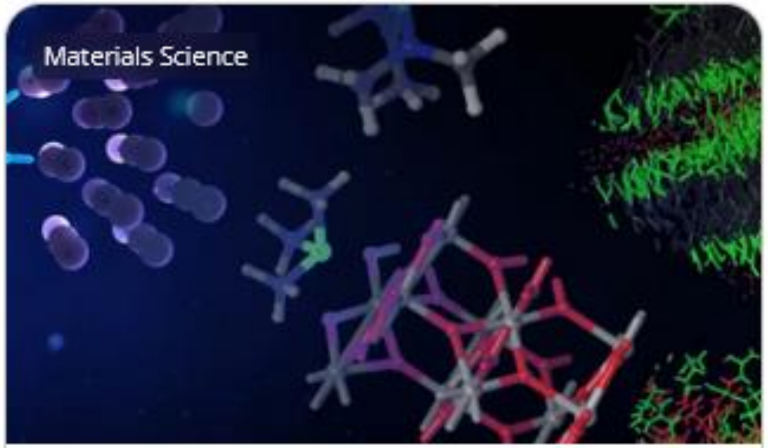
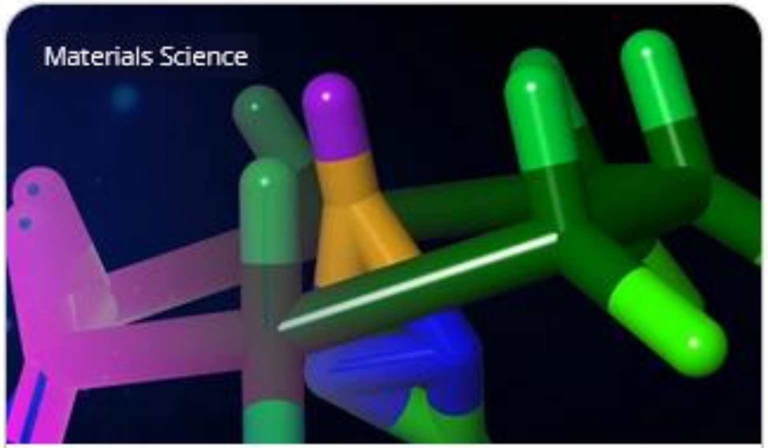




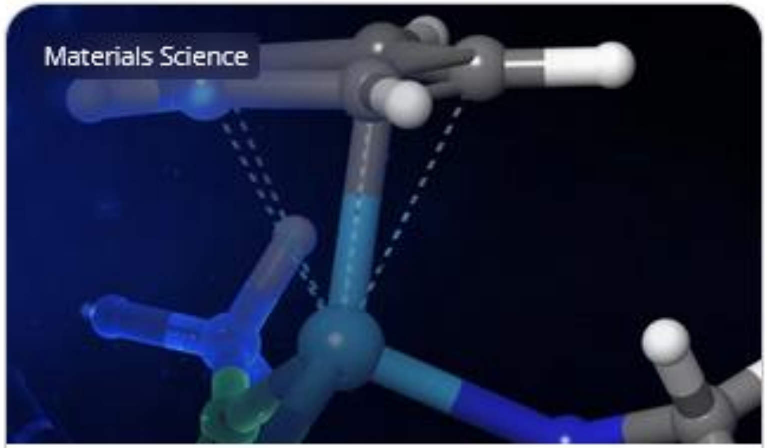
Course bundle

Access all materials science courses with a single, discounted registration



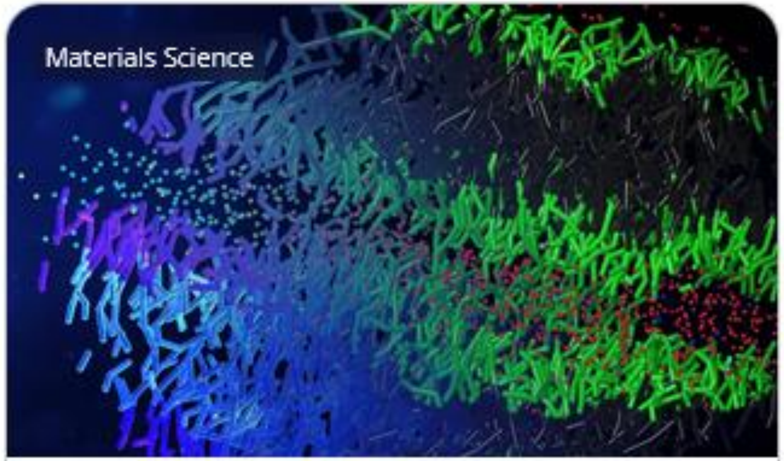
Pharmaceutical formulations

Molecular and periodic quantum mechanics, all atom molecular dynamics, and coarse-grained approaches for studying active pharmaceutical ingredients and their formulations



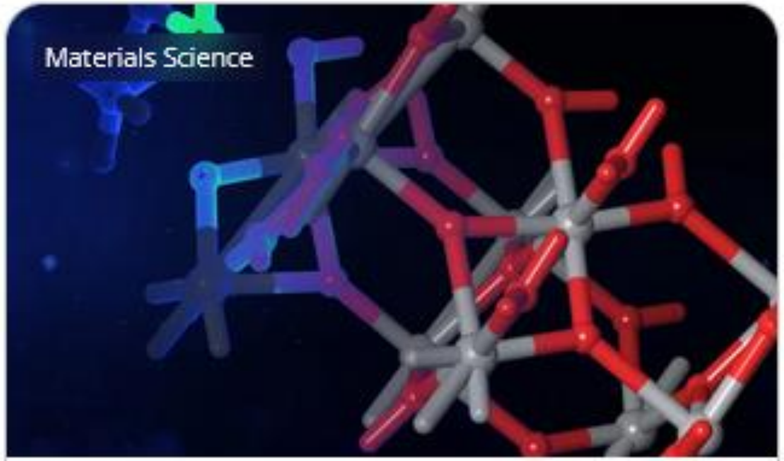
Homogeneous catalysis and reactivity

Molecular quantum mechanics and machine learning approaches for studying reactivity and mechanism at the molecular level



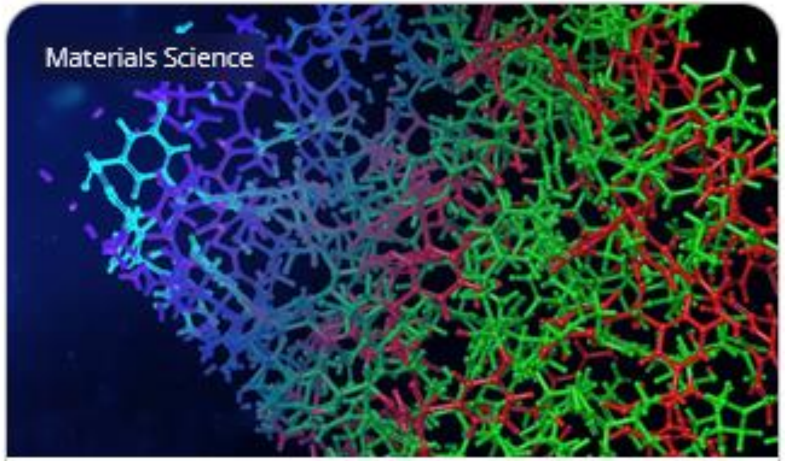
Consumer packaged goods

All-atom molecular dynamics, coarse-grained, and machine learning approaches for studying materials integral to the formulation of CPG



Surface chemistry

Molecular quantum mechanics, periodic quantum mechanics, and machine learning approaches for studying atomic layer processing and heterogeneous catalysis

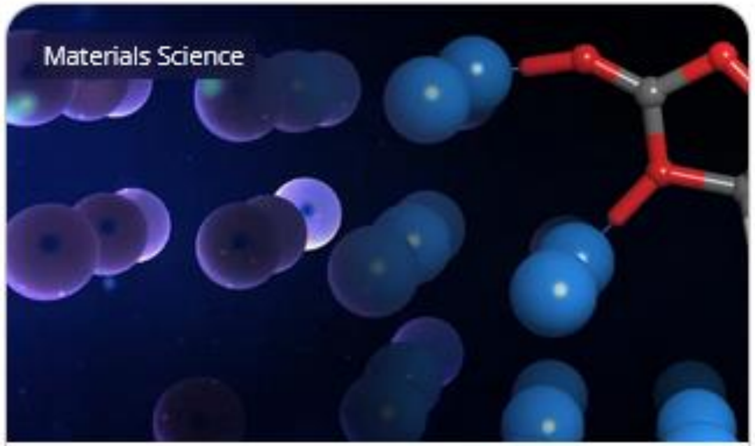


Polymeric materials

All-atom molecular dynamics and machine learning approaches for studying polymeric materials and their properties under various conditions

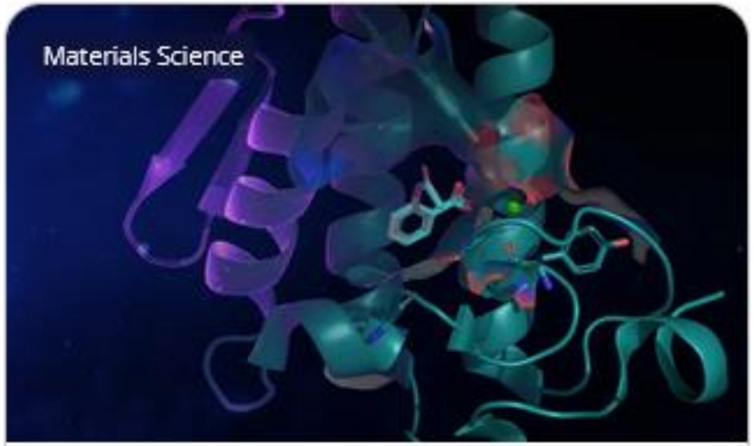
Organic electronics

Molecular quantum mechanics, all-atom molecular dynamics, and machine learning approaches for studying challenges in OLED design and discovery



Battery materials

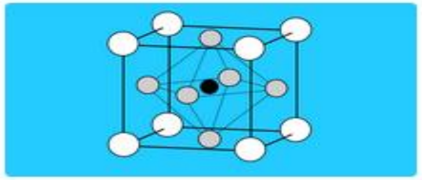
Molecular and periodic quantum mechanics, all atom molecular dynamics, and machine learning for studying battery materials and their properties under various conditions



Visualizing science with PyMOL 3

Learn how to unlock the power of movie making in PyMOL

Examples of Simulation Tools



Request Group Membership

Overview

Getting started

Materials Courses and Tutorials

Simulation-Powered Learning Activities

MSE Webinars

Online Molecular Modeling Courses

Materials Demonstrations and Outreach Activities

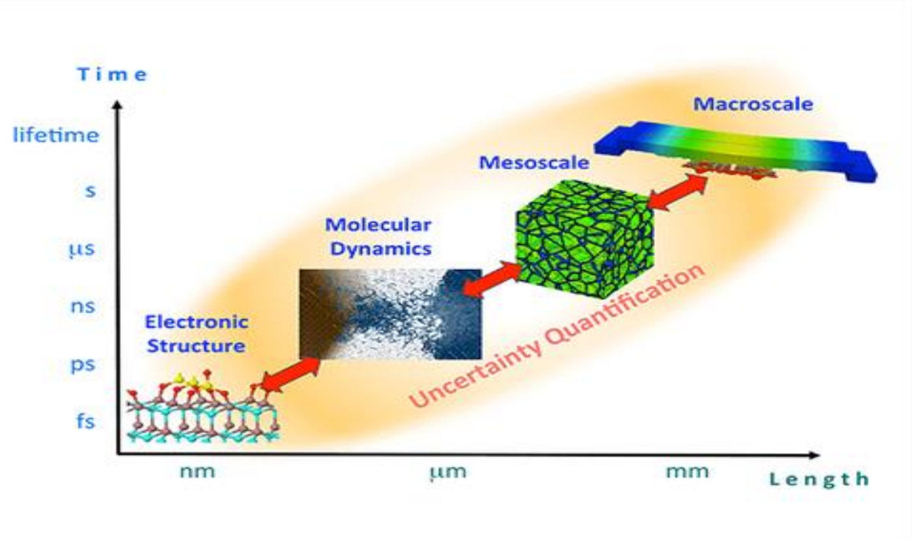
Simulation Tools

Ab Initio and Electronic

Simulation Tools

computational materials science · materials properties · materials science · materials science education · NCN Group - Materials Science

Click on a category of tools to go to a list of the corresponding tools.



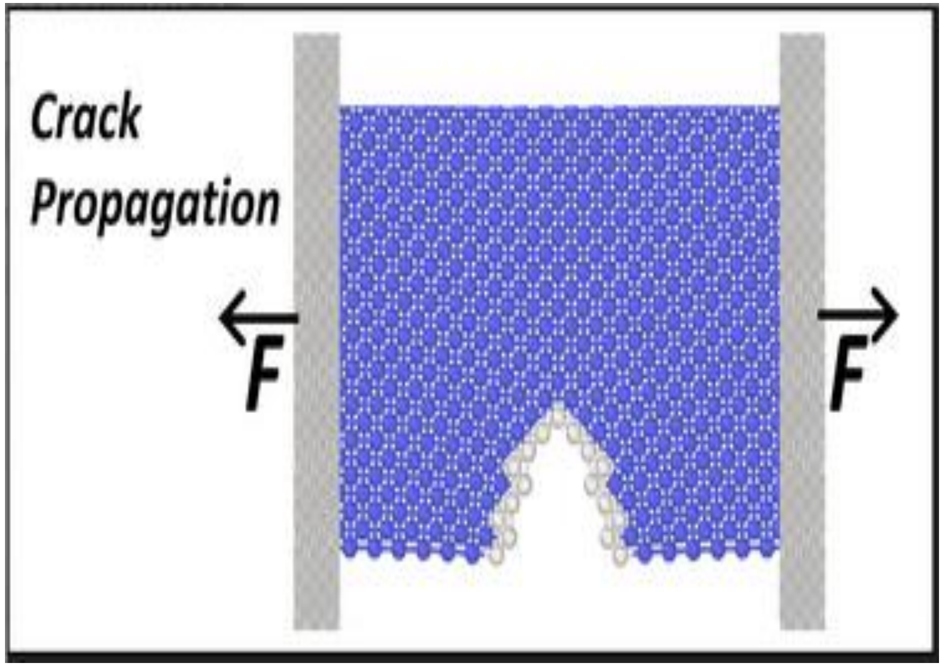
You can also see the list of

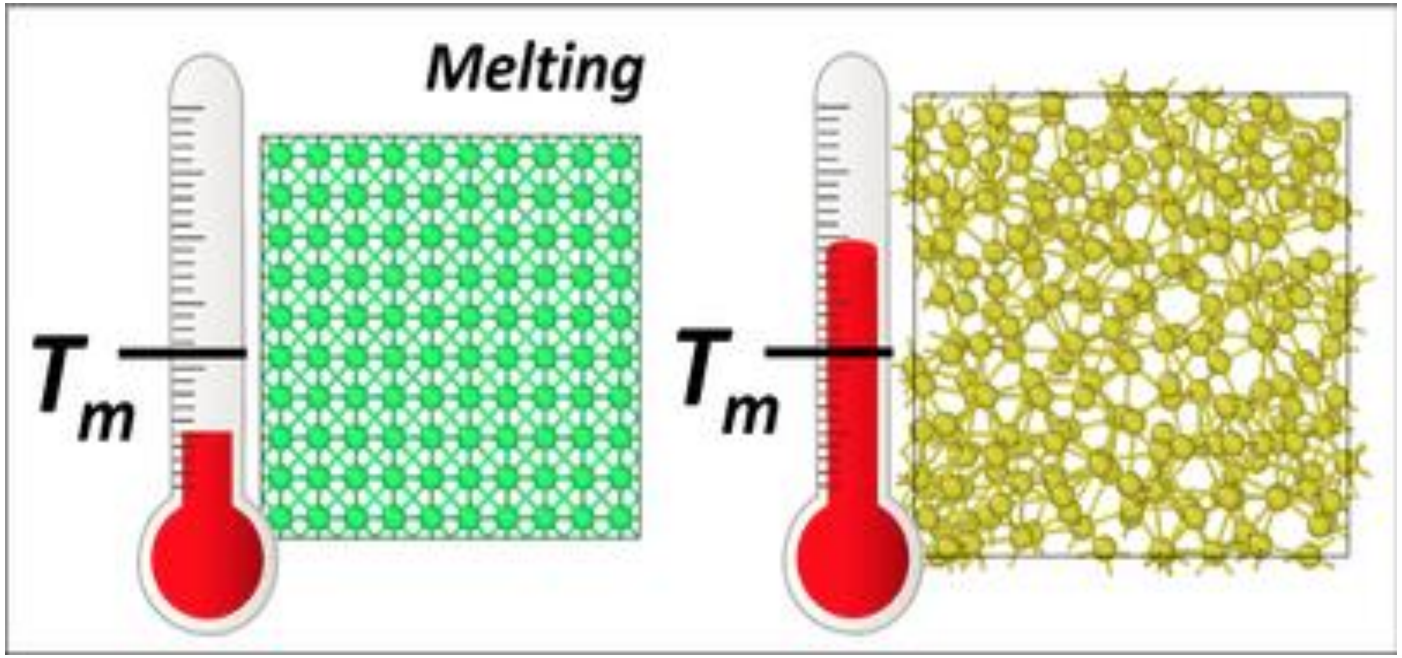
Materials Science Tool Engines and Community Codes installed in nanoHUB

Nanomaterial mechanics explorer

Examples of Simulation Tools

This tool is for those who would like to explore fundamental properties of materials such as *dislocations*, *crack propagation*, *nanowire tensile testing*, *melting* and the *martensite transformation* through atomistic Molecular Dynamics simulations.





Examples of Simulation Tools

Nanomaterial mechanics explorer

This tool is for those who would like to explore fundamental properties of materials such as *dislocations*, *crack propagation*, *nanowire tensile testing*, *melting* and the *martensite transformation* through atomistic Molecular Dynamics simulations.

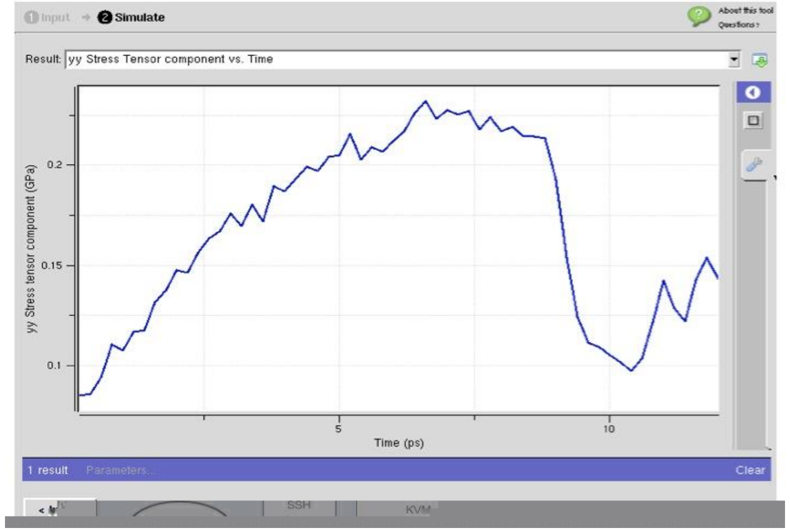
This set of tools will allow you to:

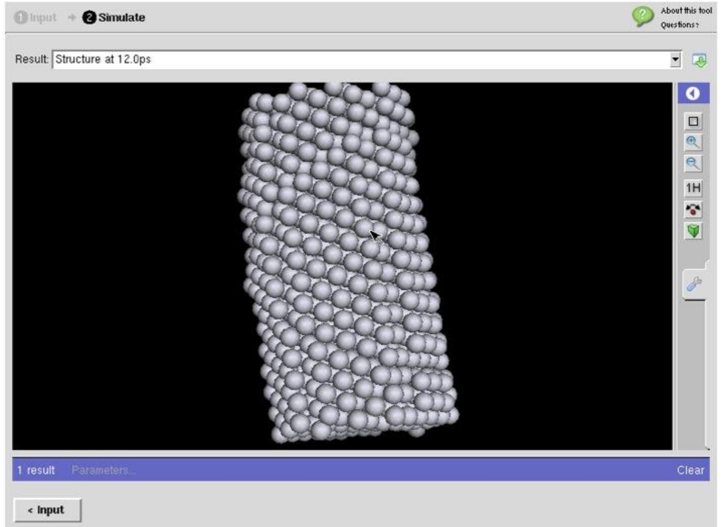
- visualize how dislocations either glide or nucleate in a crystal based on the applied stress direction relative to the Burgers vector, slip plane, and dislocation line.
- visualize how a nanowire deforms under uni-axial tensile loading, observe the process of yielding and necking, and simulate values of key engineering parameters such as the Young's modulus and yield stress. Visualize a defect in a Nickel(FCC) or Tantalum(BCC) that under uniaxial tension grows into a crack that will cause brittle fracture. Stress-strain curve, yield stress and yield strain are generated, and advanced options allow study of the brittle to ductile transition in BCC metals.
- visualize melting at the atomic level, and generate a radial distribution function. The effect of pressure on melting temperature can be studied.
- visualize a fast quench of two Ni-Al alloys, and identify the martensite transformation

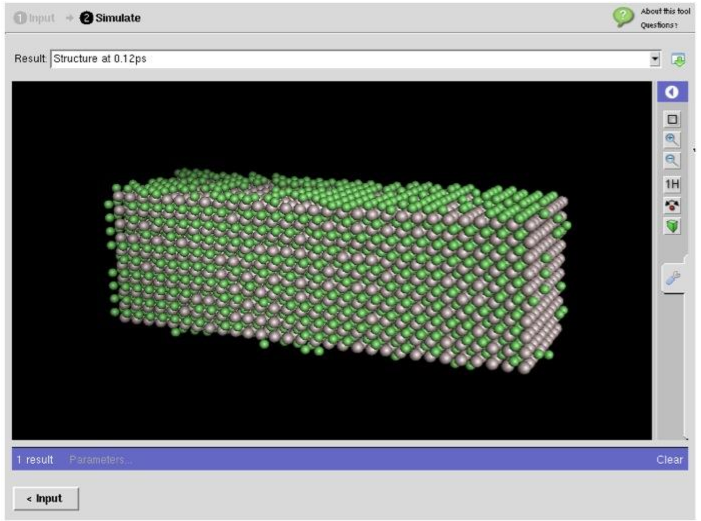
[nano-Materials Simulation Toolkit](#)

Examples of Simulation Tools

The nanoMATERIALS simulation toolkit enables users to perform molecular dynamics simulations of materials using a variety of force fields as well as electronic structure calculations



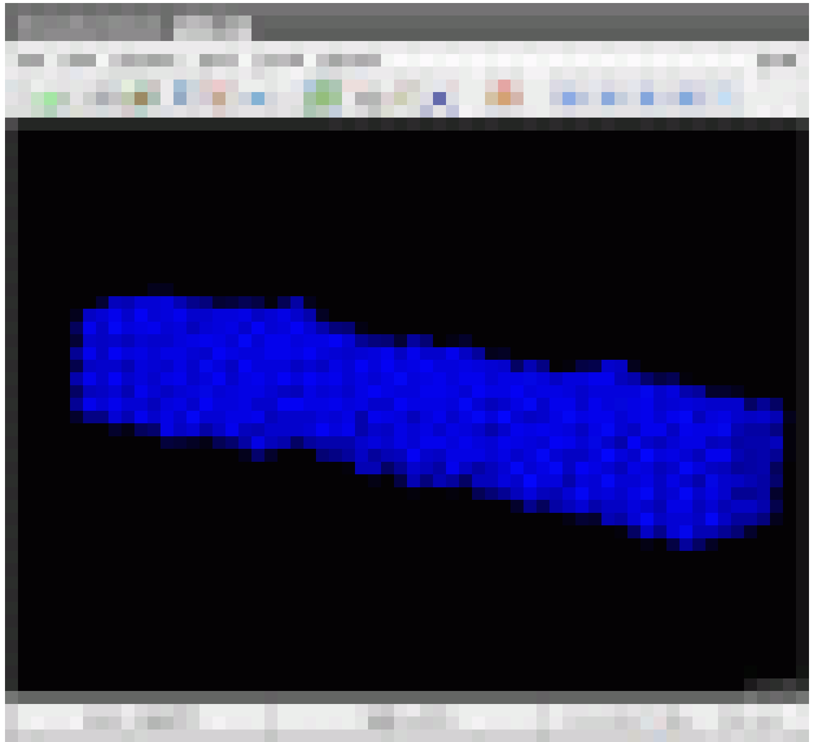




Examples of Simulation Tools

Learning Module— Atomic Picture of Plastic Deformation in Metals

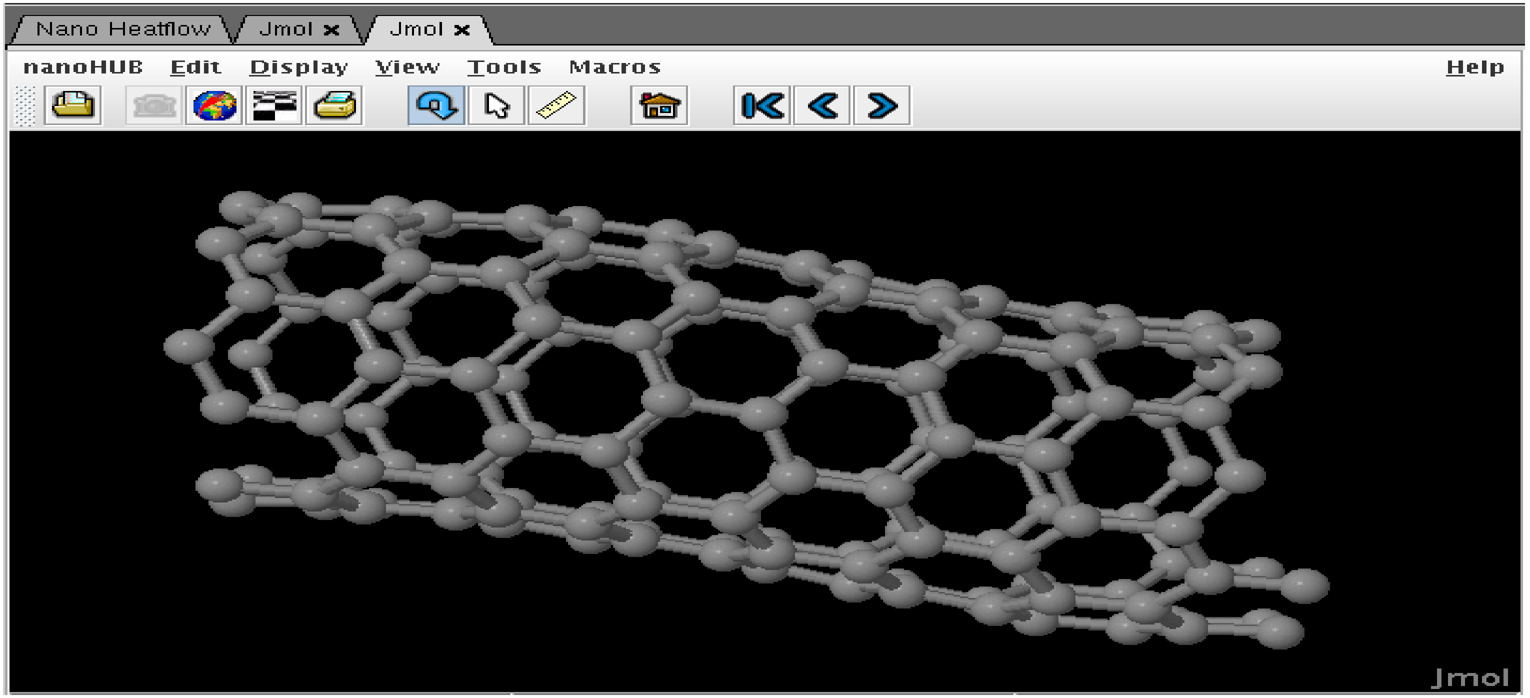
This learning module describes how this simulation tool can be used to teach concepts about plastic deformation to sophomore-level MSE students.



Examples of Simulation Tools

nanoMATERIALS nanoscale heat transport

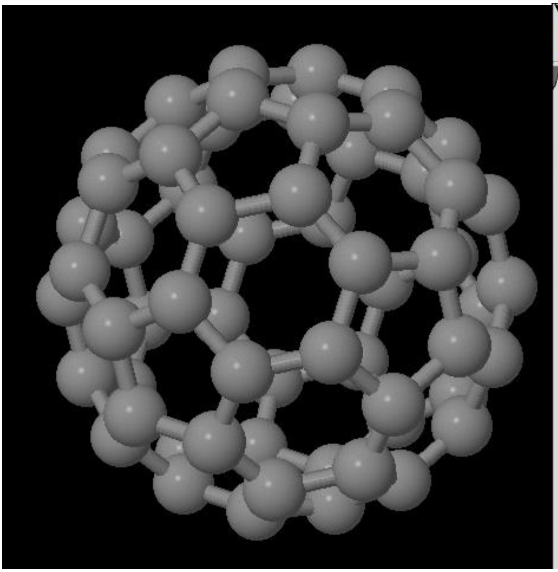
This tool will enable the users to calculate two heat transport properties: thermal conductivity and phonon relaxation time.

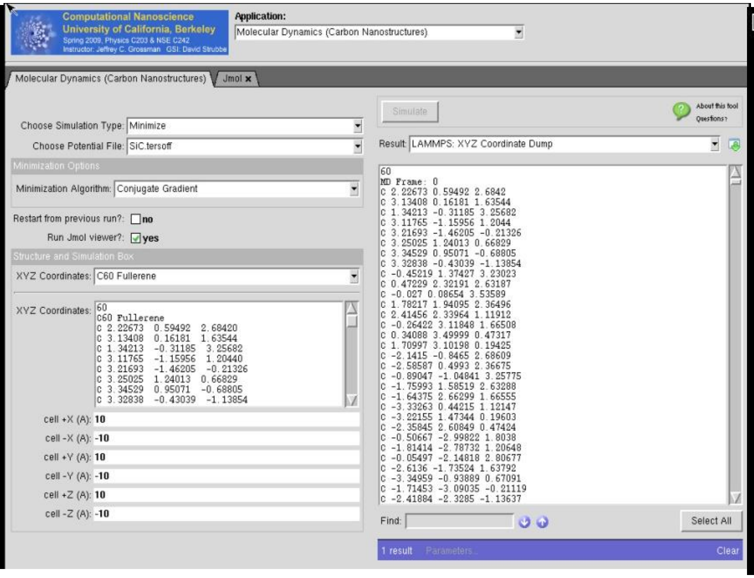


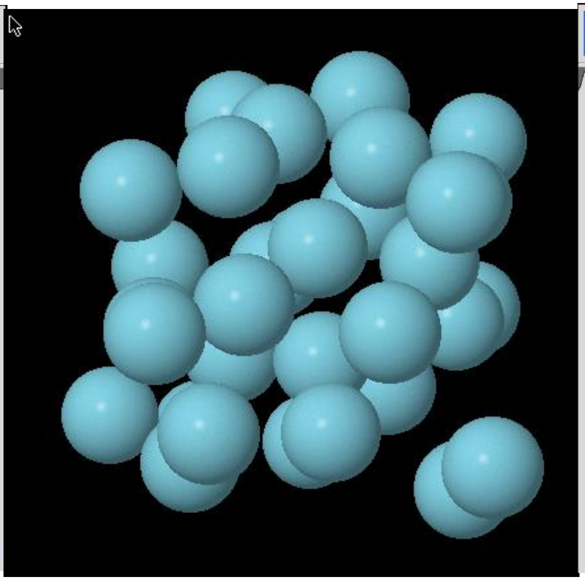
Examples of Simulation Tools

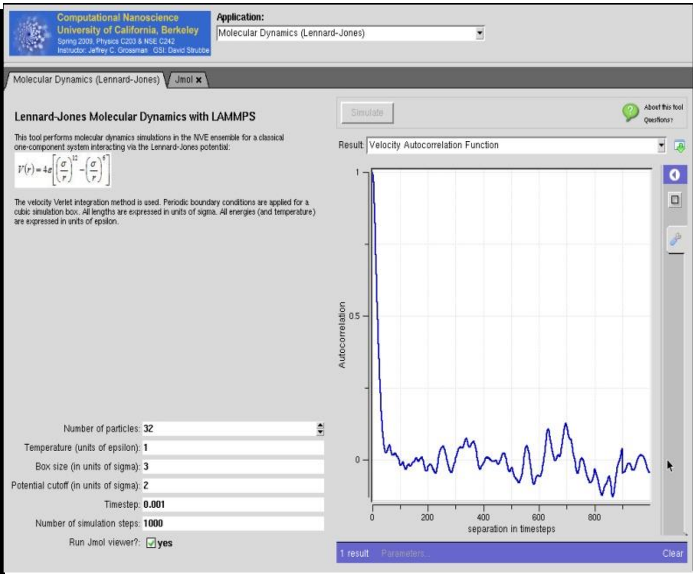
MIT Atomic-Scale Modeling Toolkit

This tool is part of MIT Atomic-Scale Modeling Toolkit which serves Overview of Computational Nanoscience: a UC Berkeley Course





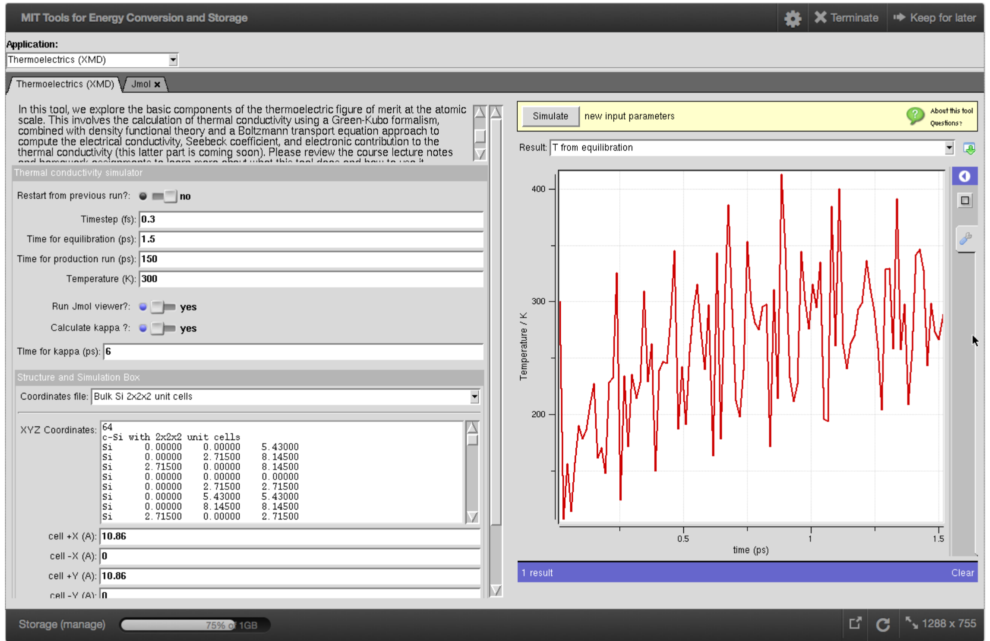


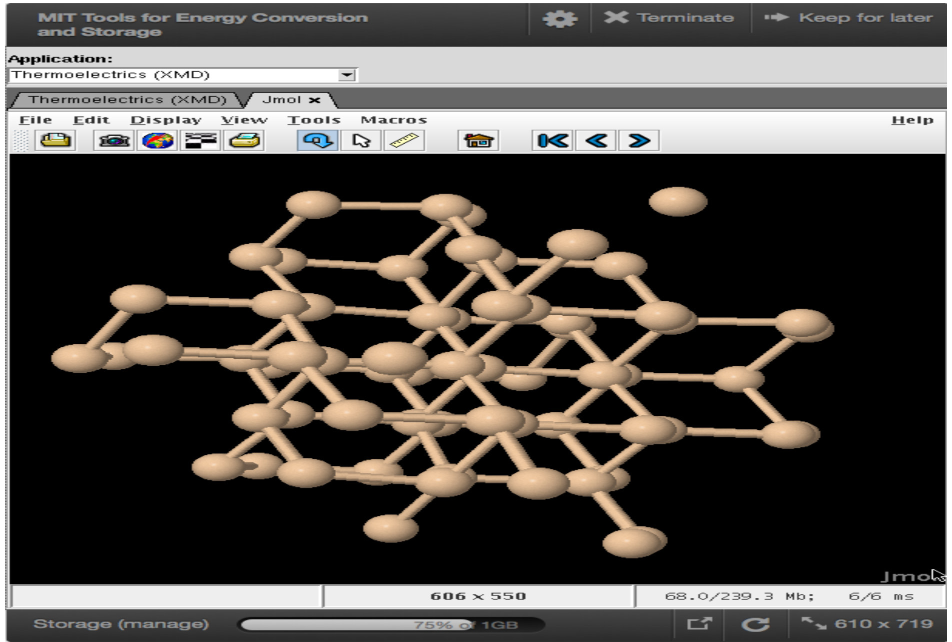


Examples of Simulation Tools

MIT Tools for Energy Conversion and Storage

These tools allow students to focus on the atomic-scale physics and chemistry underlying four separate energy conversion and storage materials: thermoelectrics, solar fuels, solar photovoltaics, and hydrogen storage. Within each of these four different tools, the user can compute properties that are directly relevant to the key fundamental conversion and storage mechanisms.

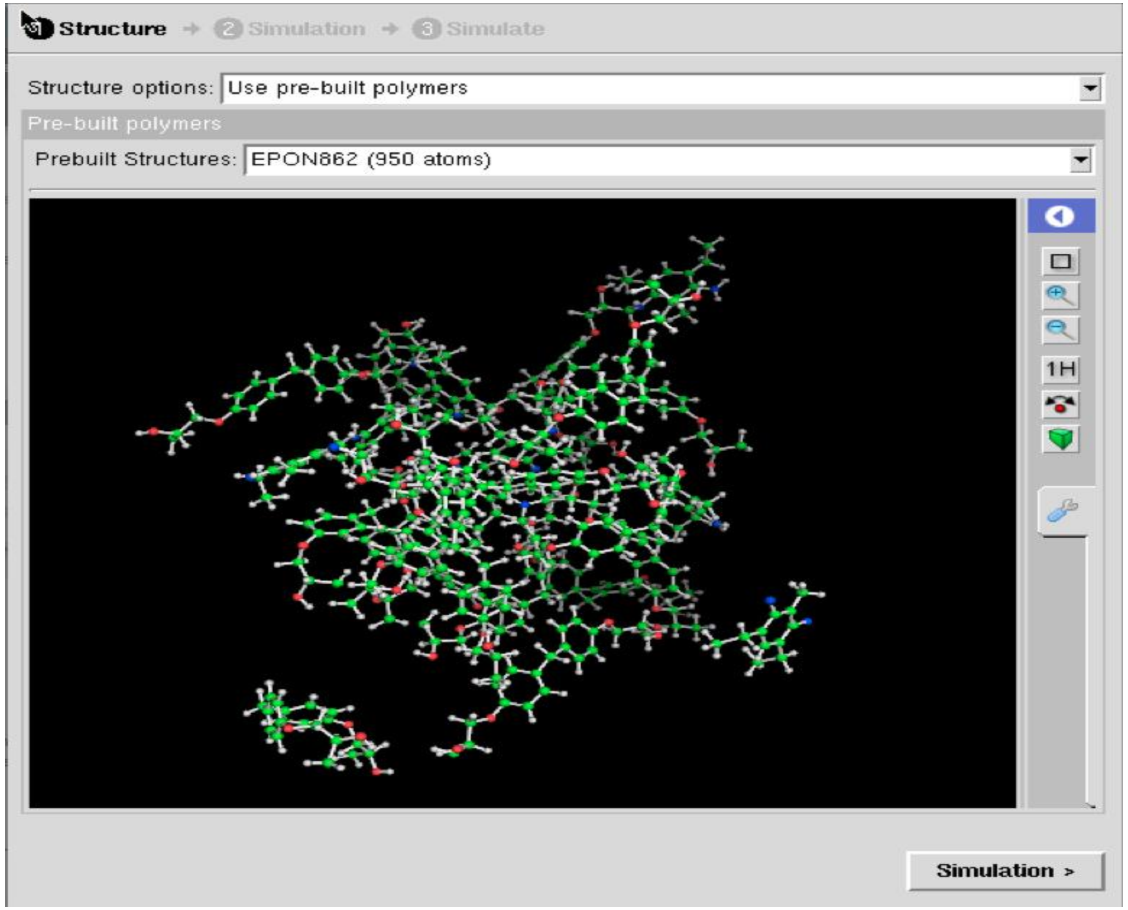




Examples of Simulation Tools

Polymatic: A Simulated Polymerization Algorithm

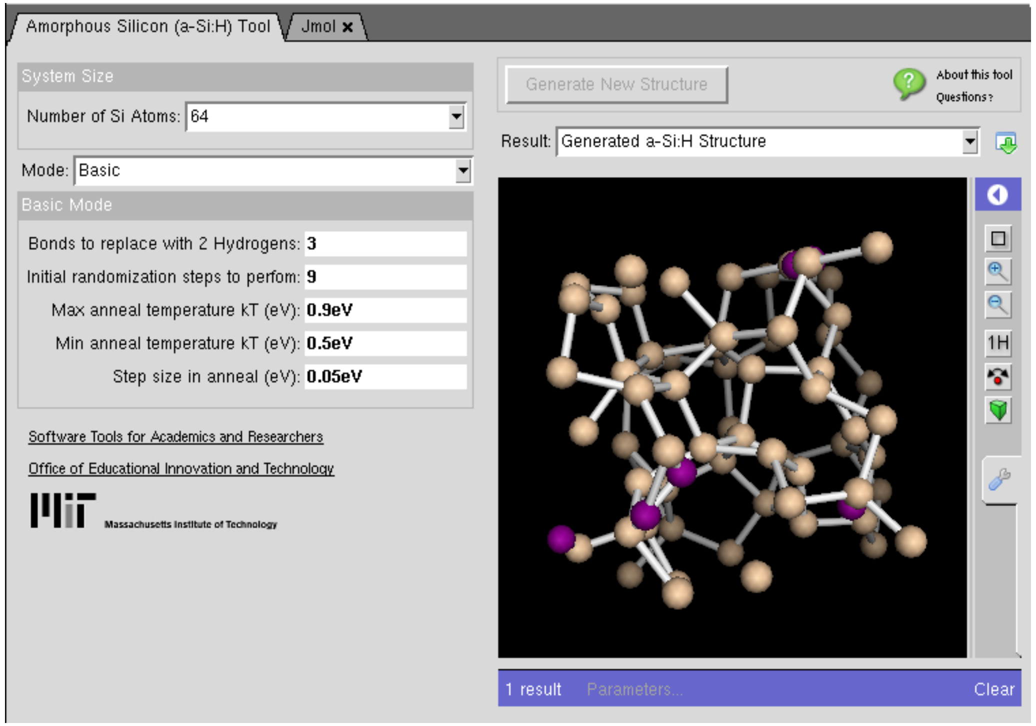
Polymatic is a set of codes for structure generation of amorphous polymers by a simulated polymerization algorithm. The main task of Polymatic is to perform polymerization steps within a system based on a number of defined bonding criteria. It works in conjunction with a simulation package to perform energy minimization and molecular dynamics simulations during the polymerization.



Examples of Simulation Tools

Amorphous Silicon Generator

This tool generates realistic random-network models of a-Si with periodic boundary conditions.



Examples of Simulation Tools

Molecular Dynamics with Monte Carlo Simulations

RASPA tools, which include:

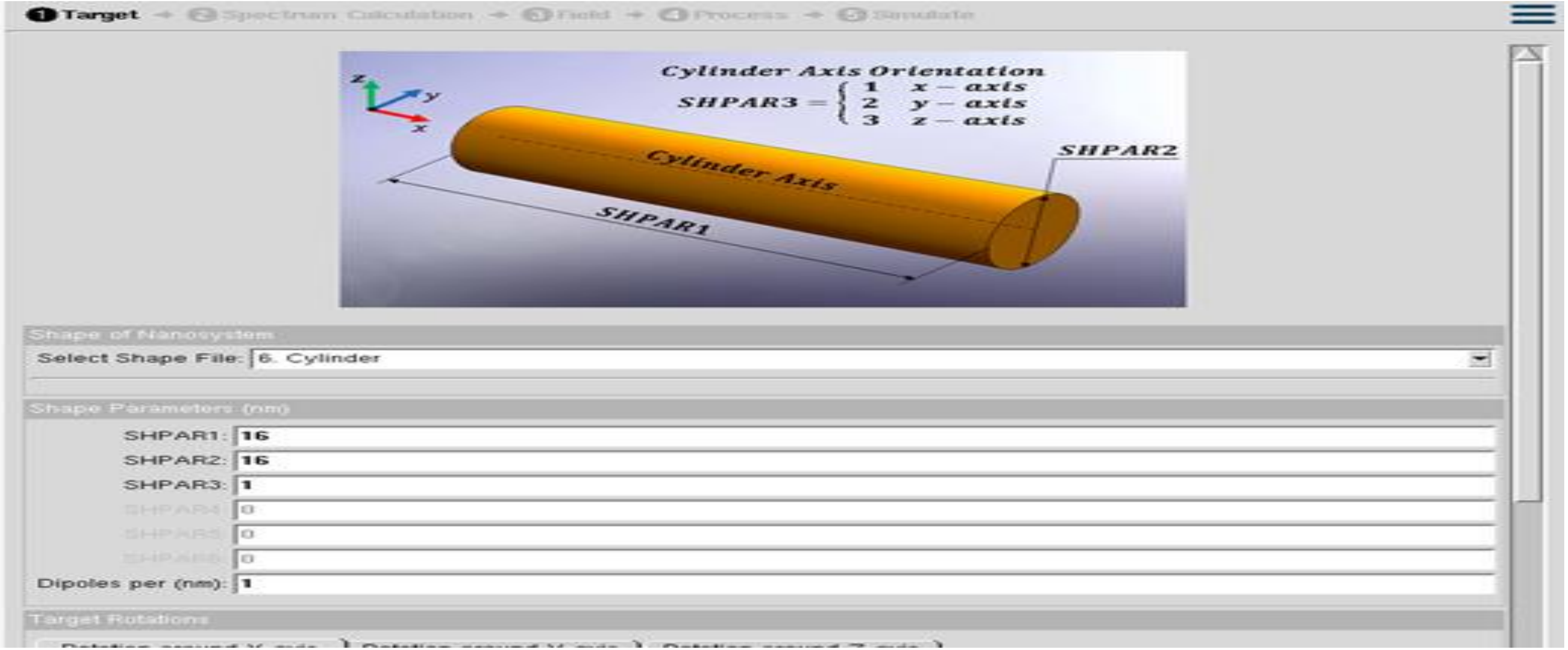
- Void Fraction Calculator
- Calculates the void fraction (pore volume) of nano-porous materials
- Gibbs Adsorption Simulator
    - Simulates the adsorption of gases using Gibbs ensemble
- Adsorption Energy Calculator
    - Calculate the total energy of adsorbates as they move around a metal organic framework
- Gas Adsorption Calculator
    - Simulates gas adsorption onto metal organic frameworks
- Henry Coefficient Simulator
    - Calculate Henry's constant of several sites on a nanoporous material
- Gas Diffusion Coefficient in Metal Organic Frameworks
    - Calculates gas self diffusion coefficient in metal organic frameworks

Examples of Simulation Tools

NanoDDSCAT

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

1. Target

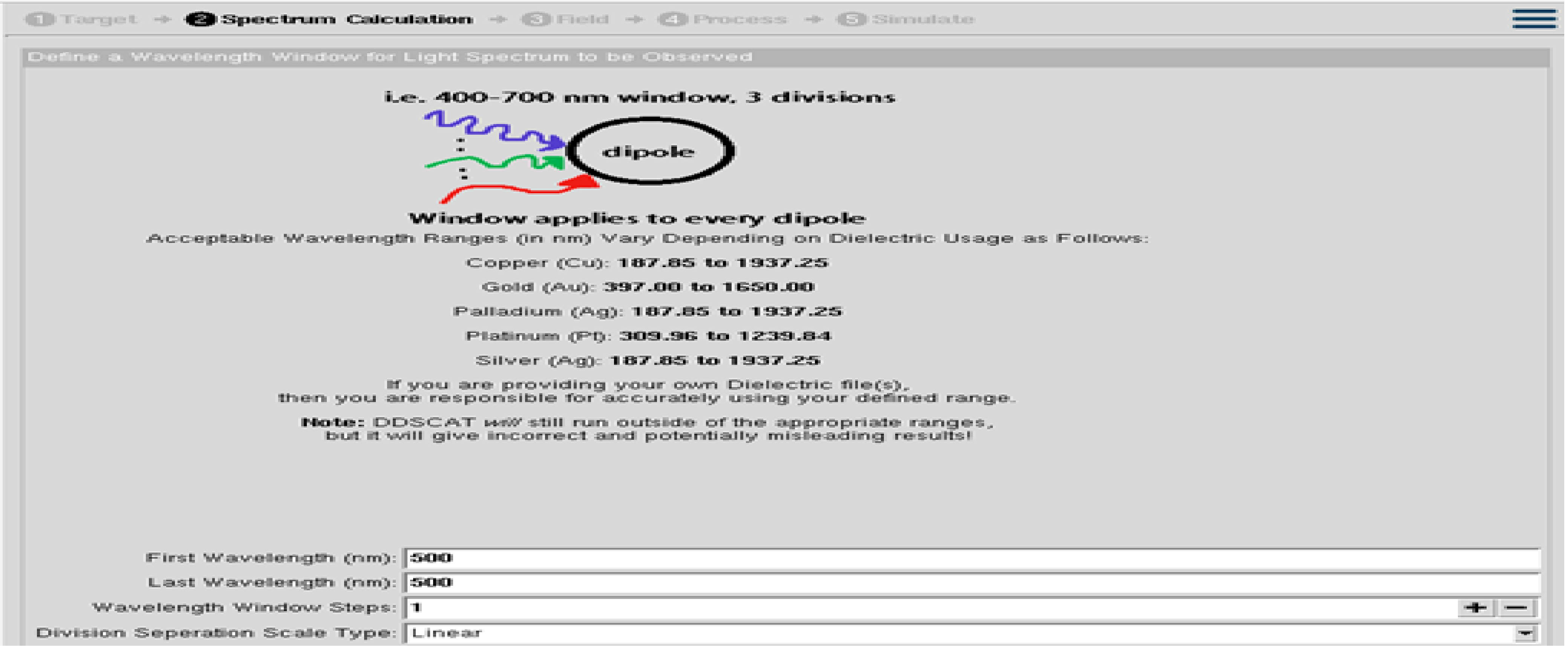


Examples of Simulation Tools

NanoDDSCAT

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

2. Spectrum Calculation

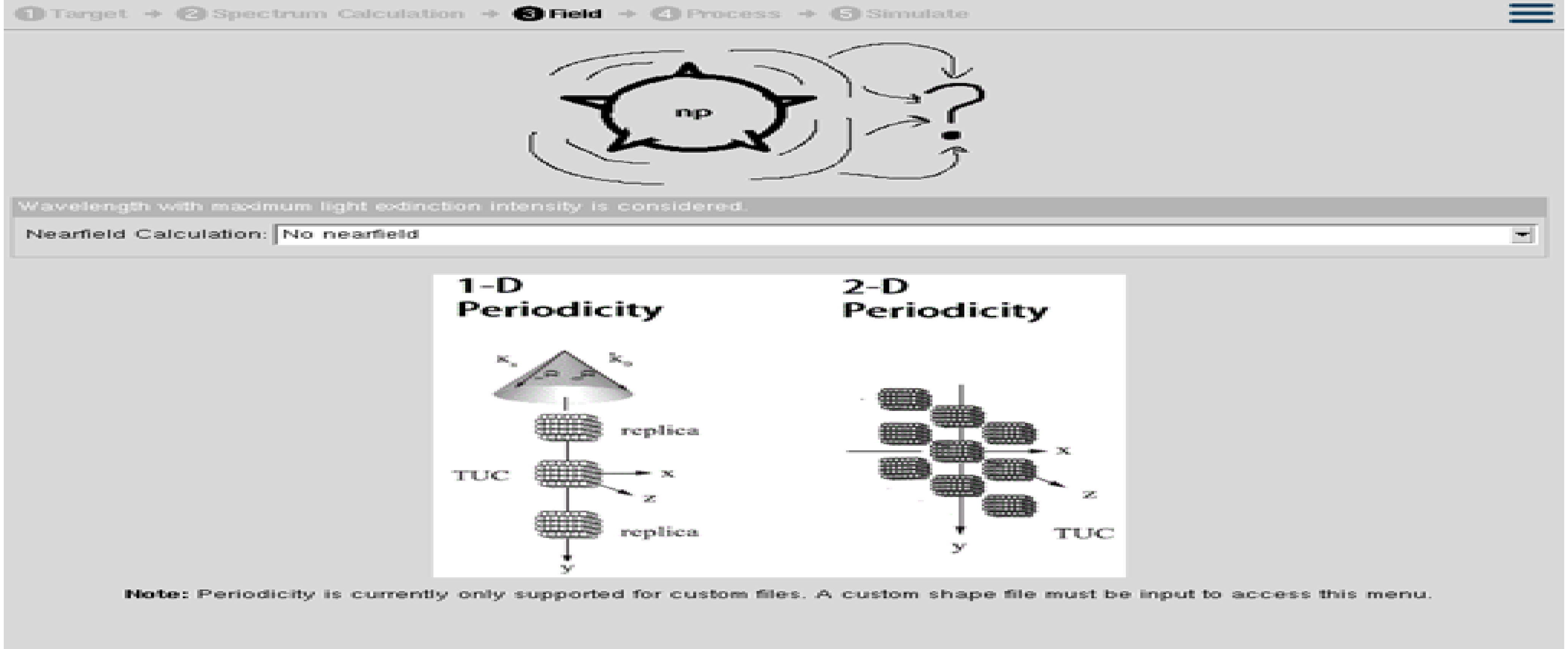


Examples of Simulation Tools

NanoDDSCAT

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

3. Field



Examples of Simulation Tools

NanoDDSCAT

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

4. Process and Simulate

NanoDDSCAT

Examples of Simulation Tools

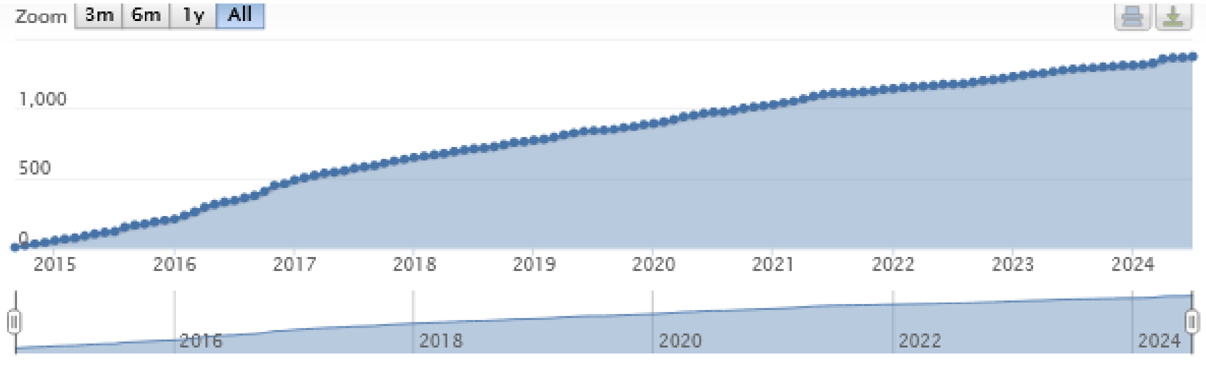
Worldwide Usage

nanoHUB

EXPLORE PUBLISH COMMUNITY ABOUT SUPPORT

Cumulative Simulation Users

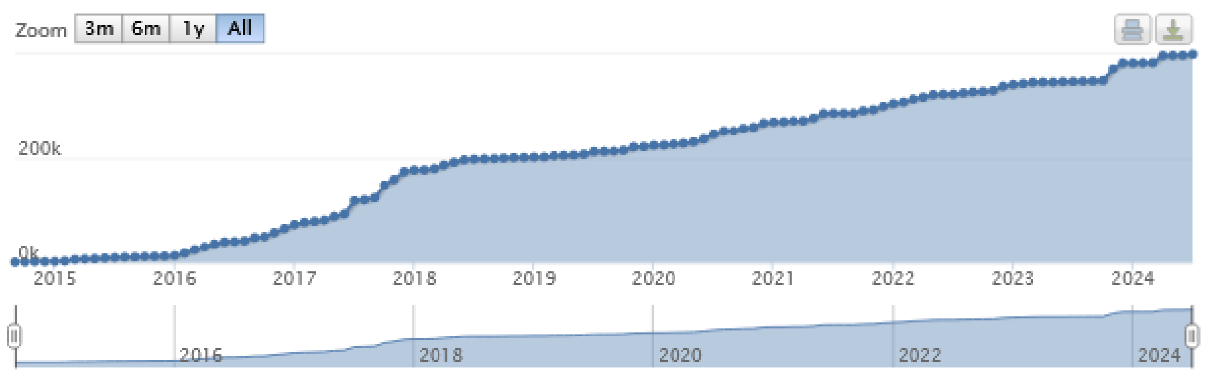
1,372



Simulation Runs

397,099

Jun 2024

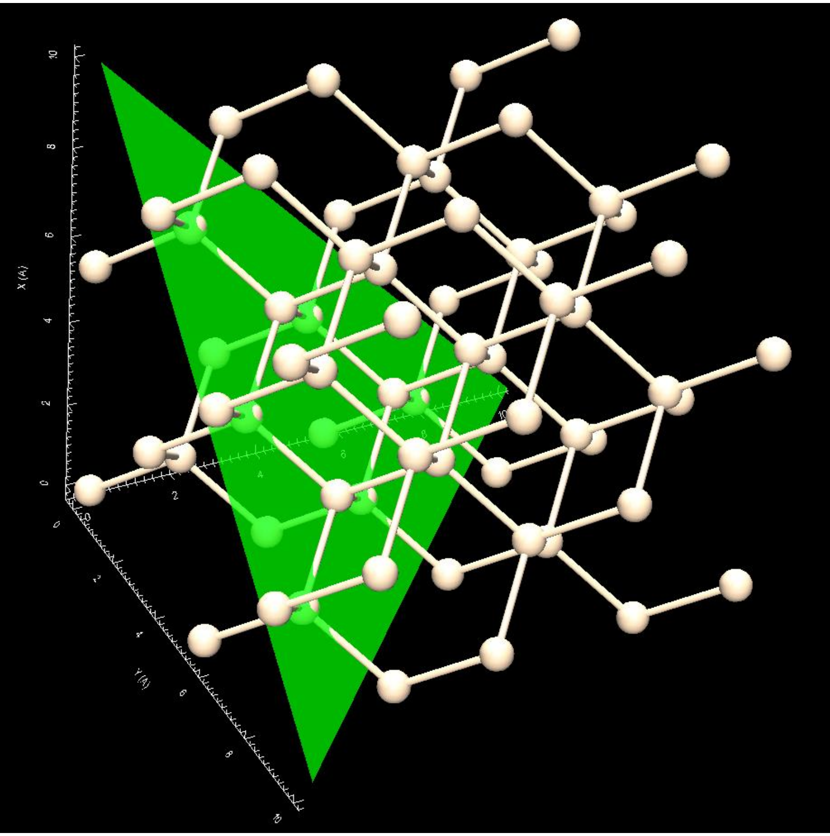


Examples of Simulation Tools

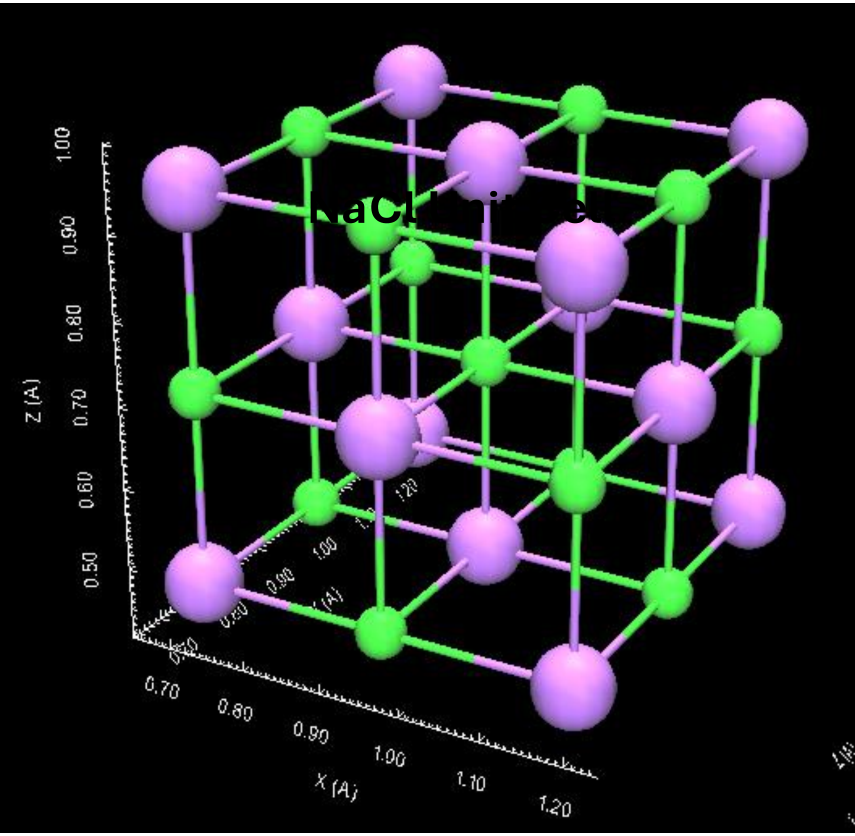
The Crystal Viewer simulation tool allows:

(a) viewing all materials which have periodical structure

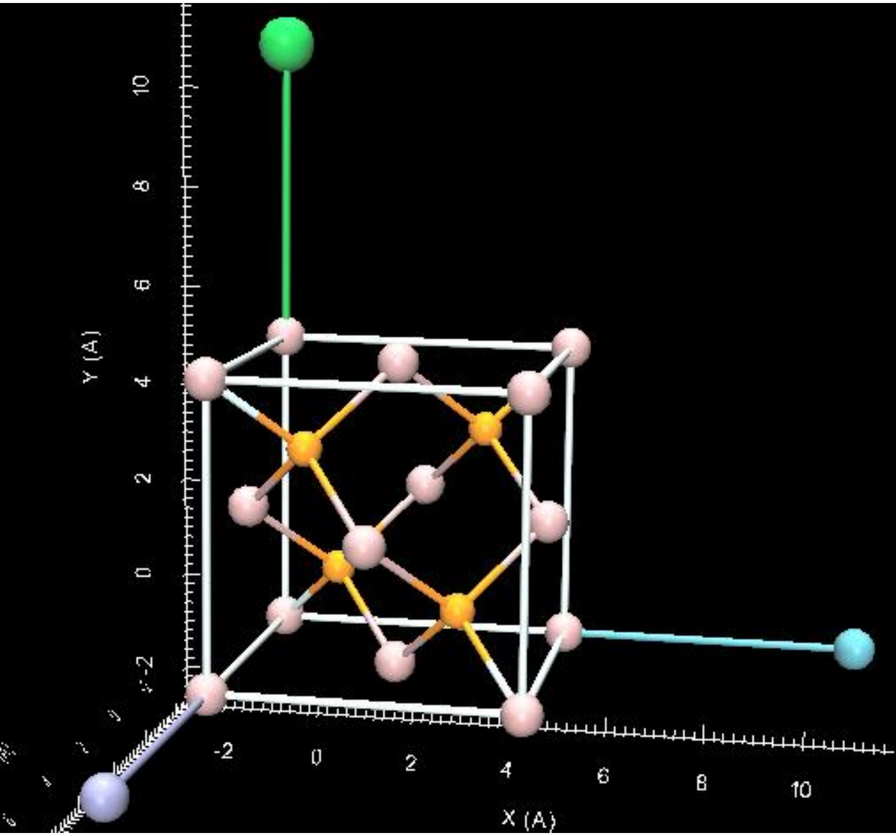
(b) building crystal structure even not exists in nature



Silicon With Miller Plane

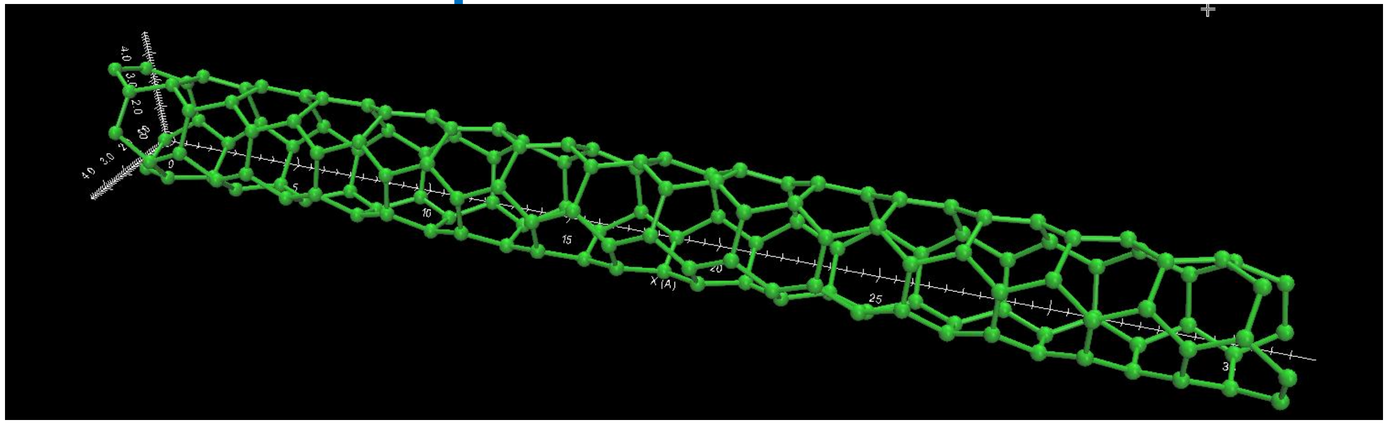


NaCl Unit Cell

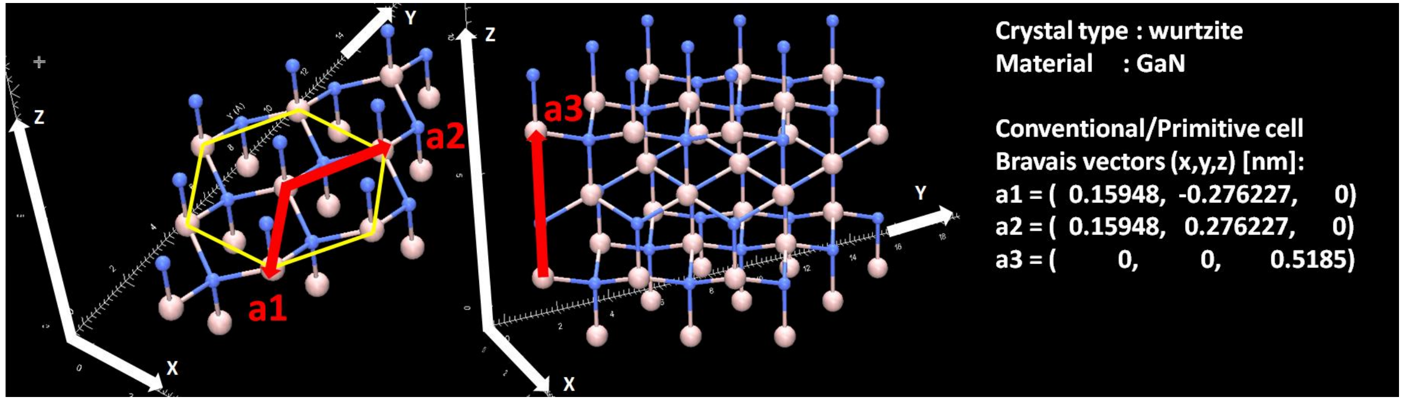


GaP Unit Cell

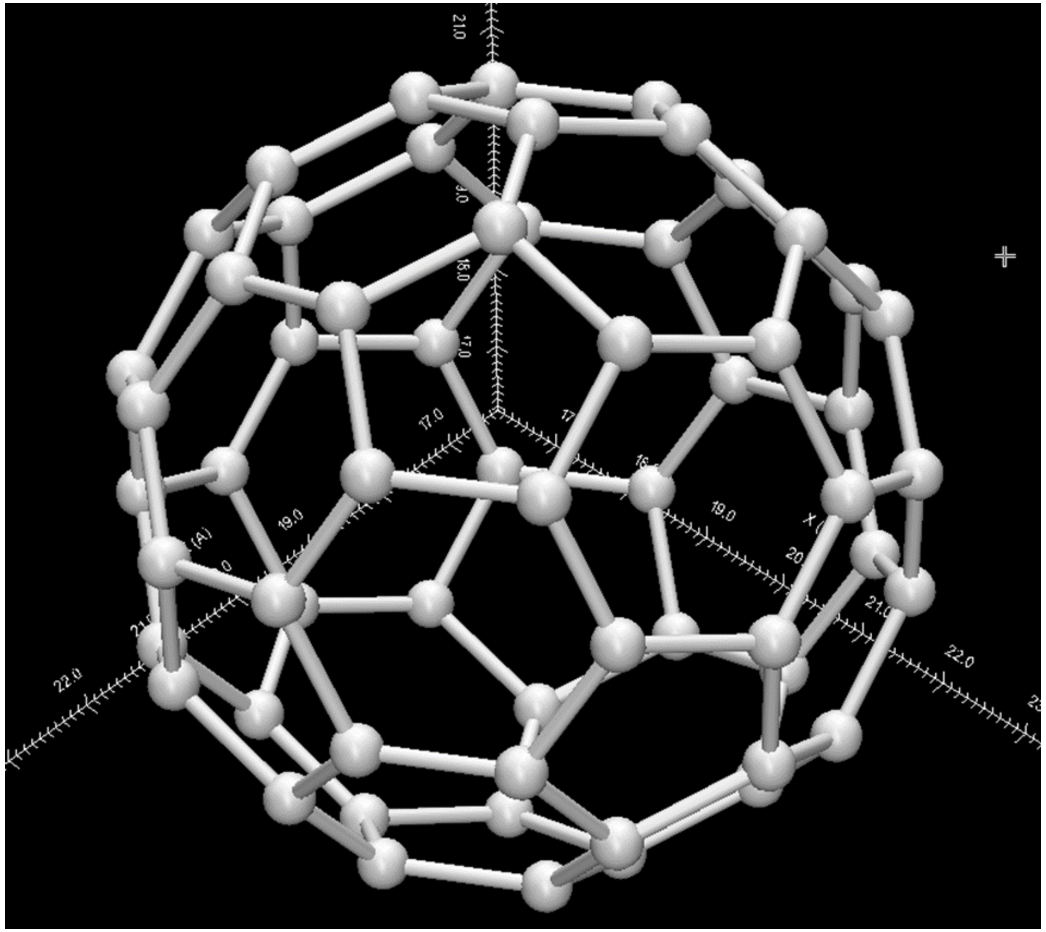
Examples of Nano Structure Visualization



Carbon nano tube



GaN Bravais Vectors



Buckey Ball

Examples of Nano Structure Visualization

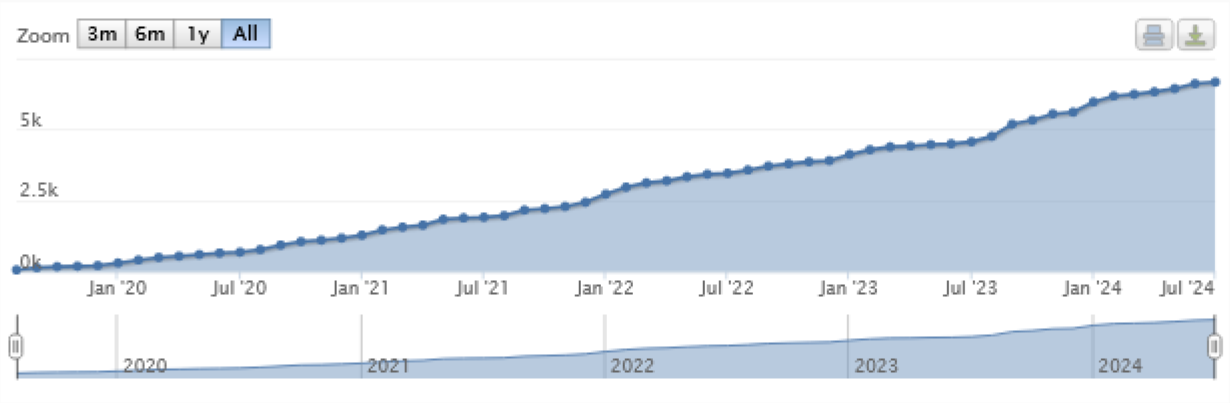
https://youtu.be/wm3VpgbM6_w

Crystal Viewer

Worldwide Usage

Cumulative Simulation Users

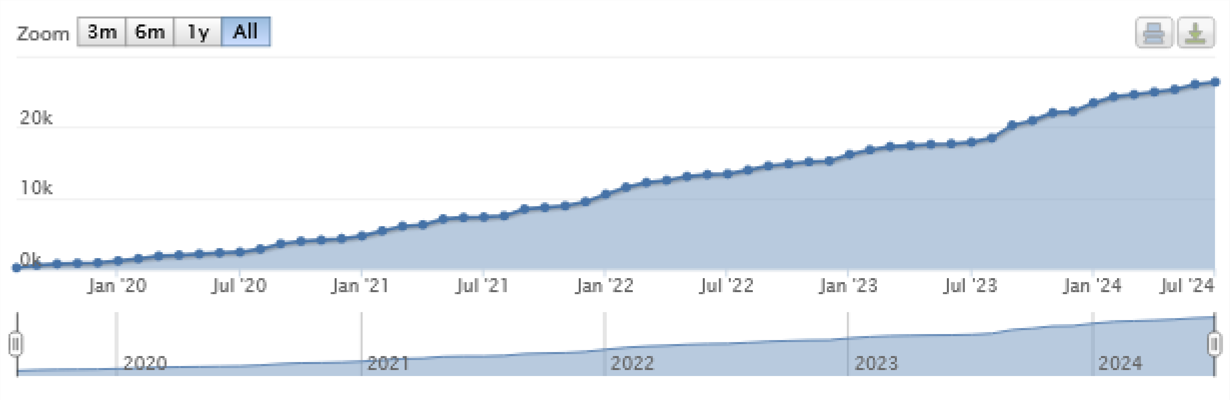
6,671



Simulation Runs

26,381

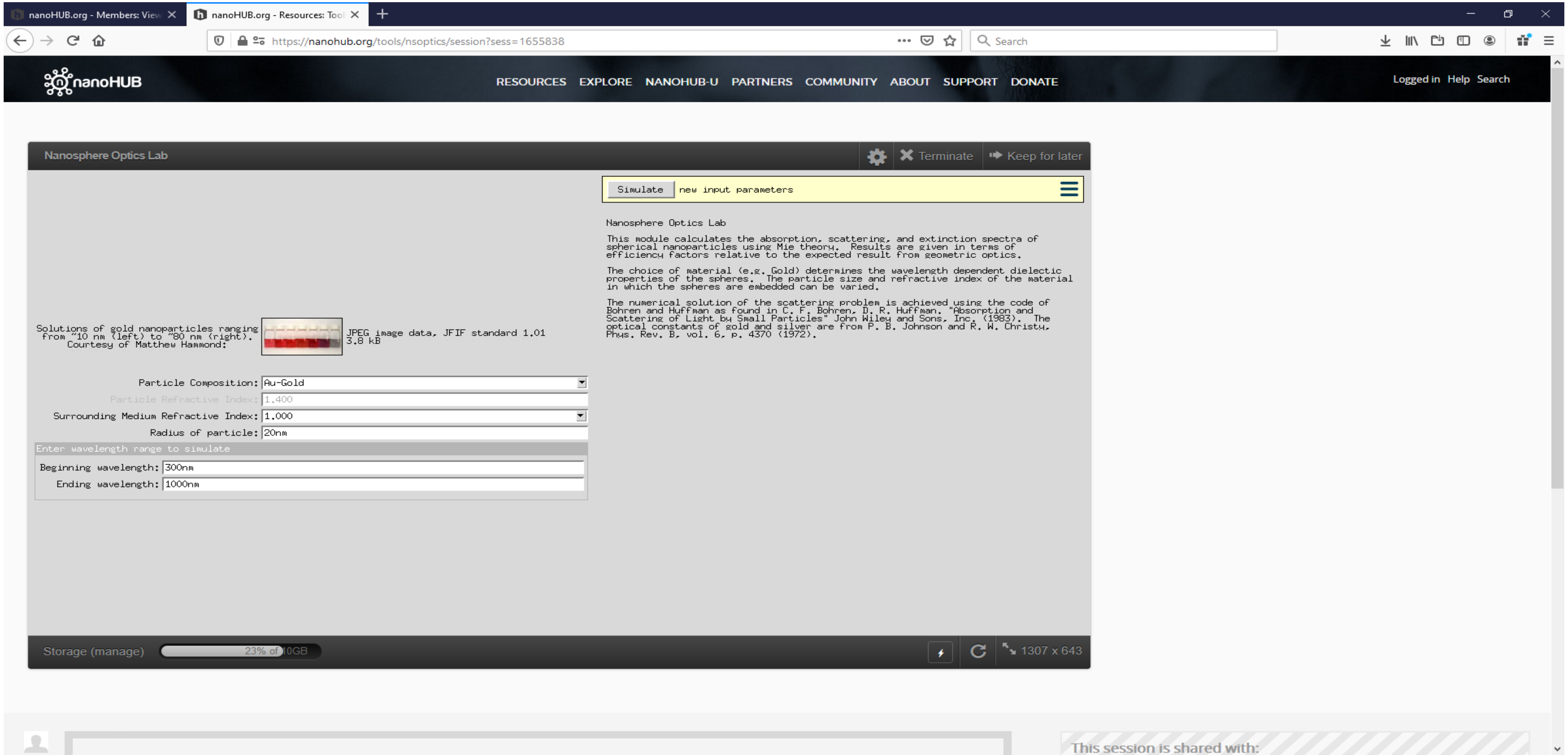
Jun 2024



Nanosphere Optics Lab over NanoHub

Examples of Simulation Tools

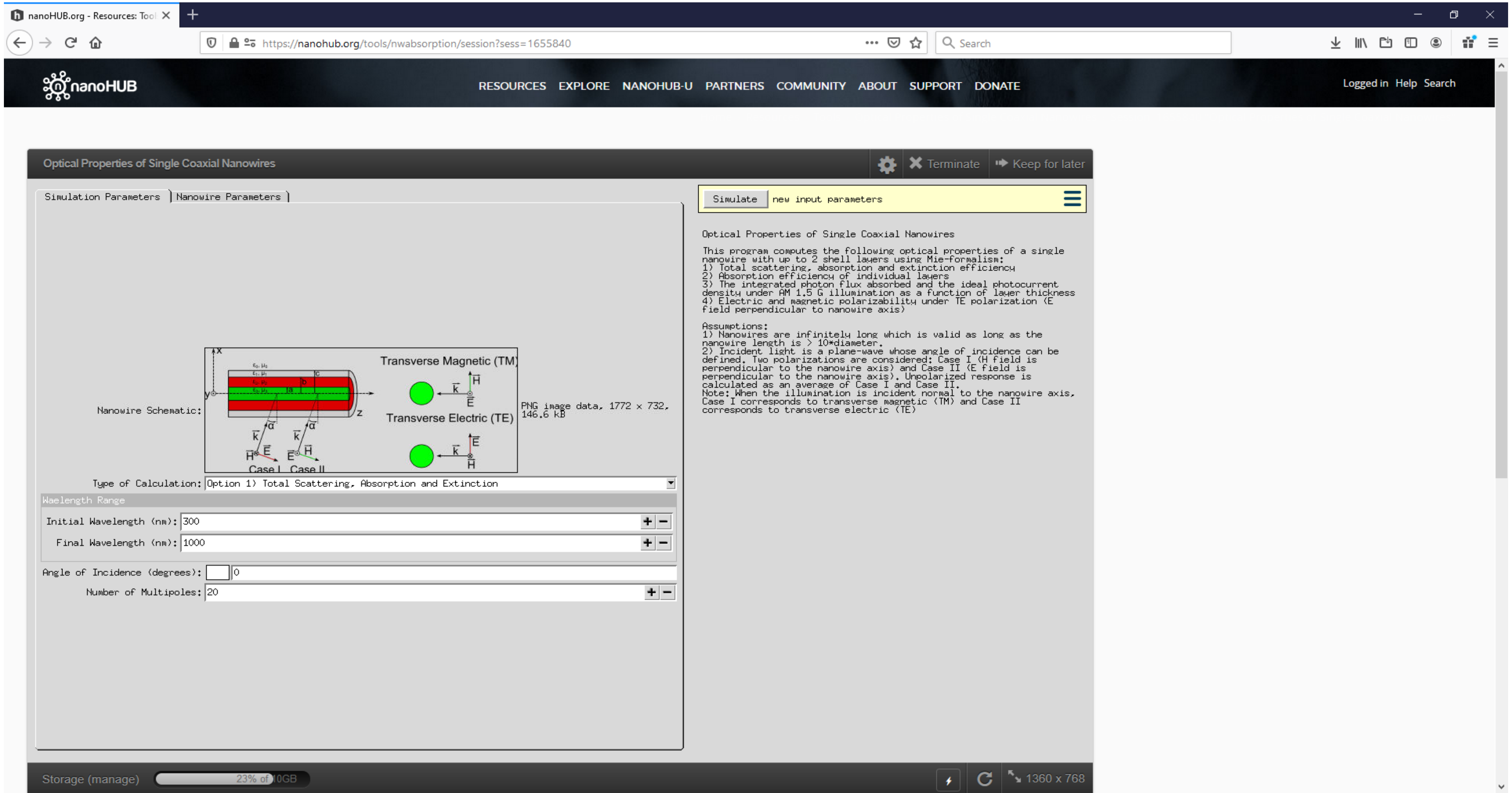
Calculate absorption from metallic nanoparticles



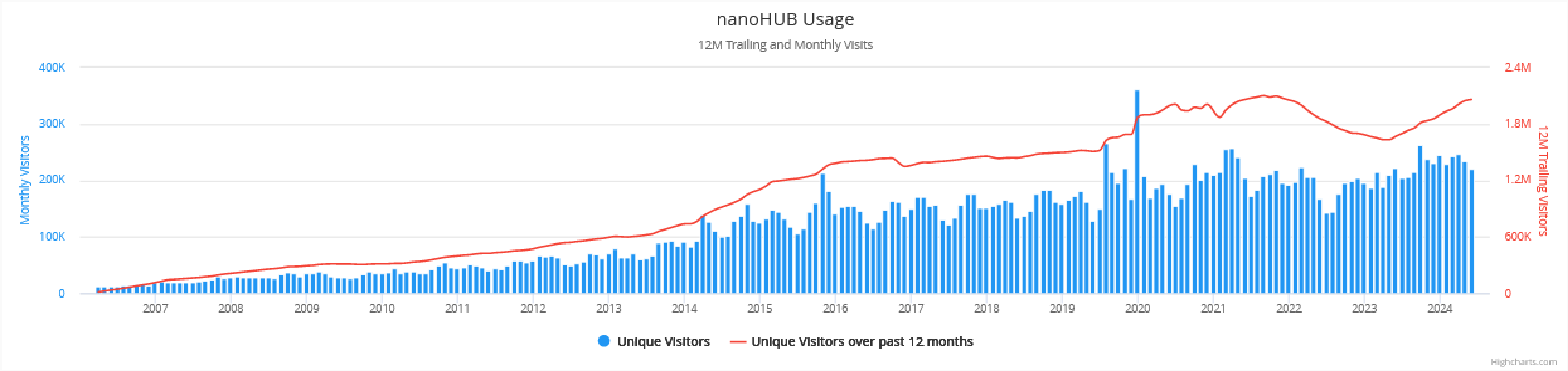
Nanosphere Optics Lab over NanoHub

Examples of Simulation Tools

Calculate absorption and scattering from single nanowires with or without shells

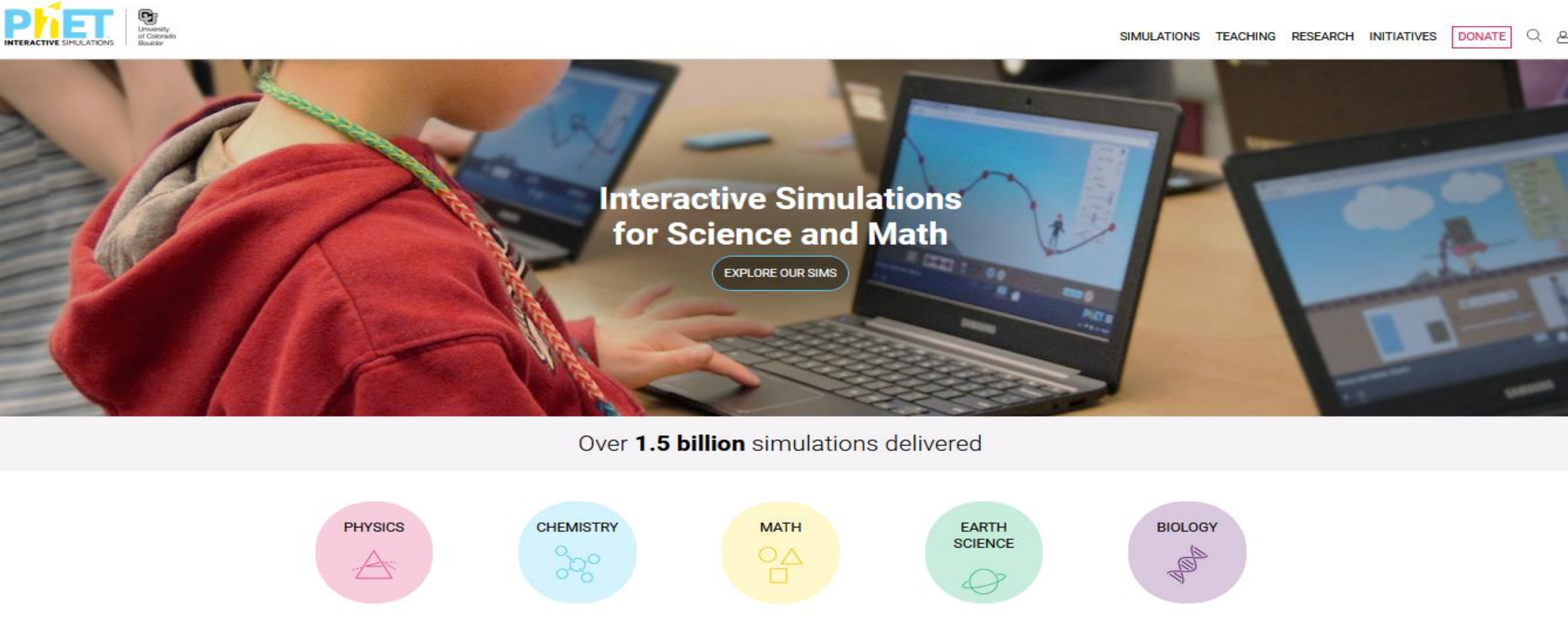


NanoHub:
Worldwide Usage



2,060,048 Unique Visitors	303,140 Registered Users
7,891 Resources	839 Published Tools
2,787 Citations	23,115 Simulation User Count


HI TEC
Preparing America's Skilled Technical Workforce
HI TEC 2024
Kansas City
15TH ANNIVERSARY
July 29—Aug 1

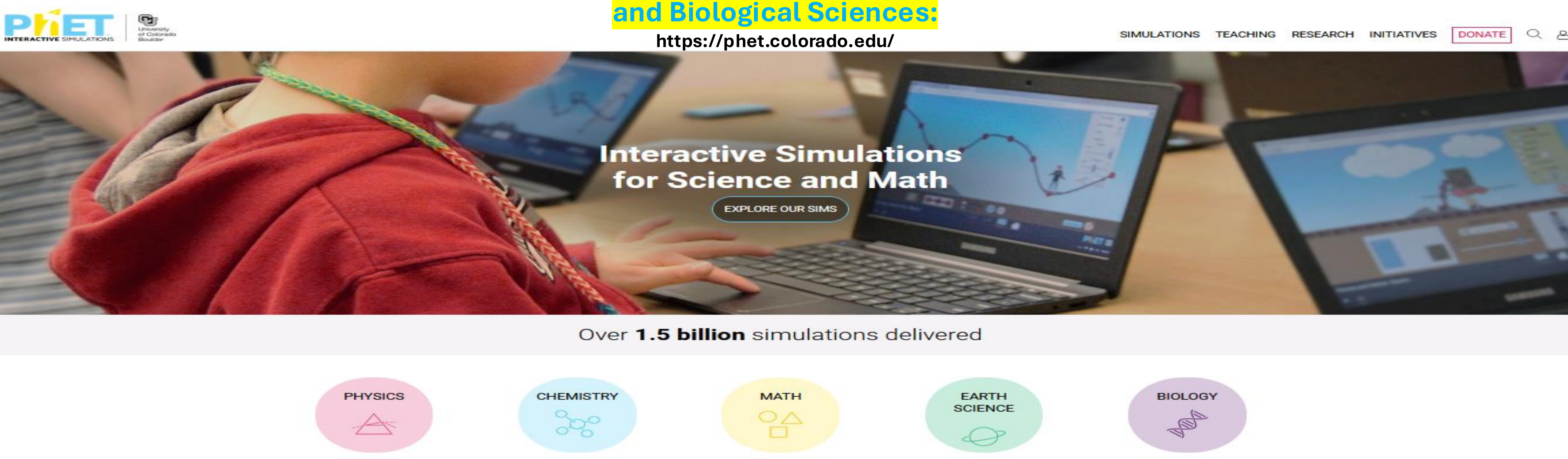

PhET INTERACTIVE SIMULATIONS
University of Colorado Boulder
SIMULATIONS
TEACHING
RESEARCH
INITIATIVES
DONATE
Interactive Simulations for Science and Math
EXPLORE OUR SIMS
Over 1.5 billion simulations delivered
PHYSICS
CHEMISTRY
MATH
EARTH SCIENCE
BIOLOGY

PhET Interactive Simulations

University of Colorado

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

https://phet.colorado.edu/

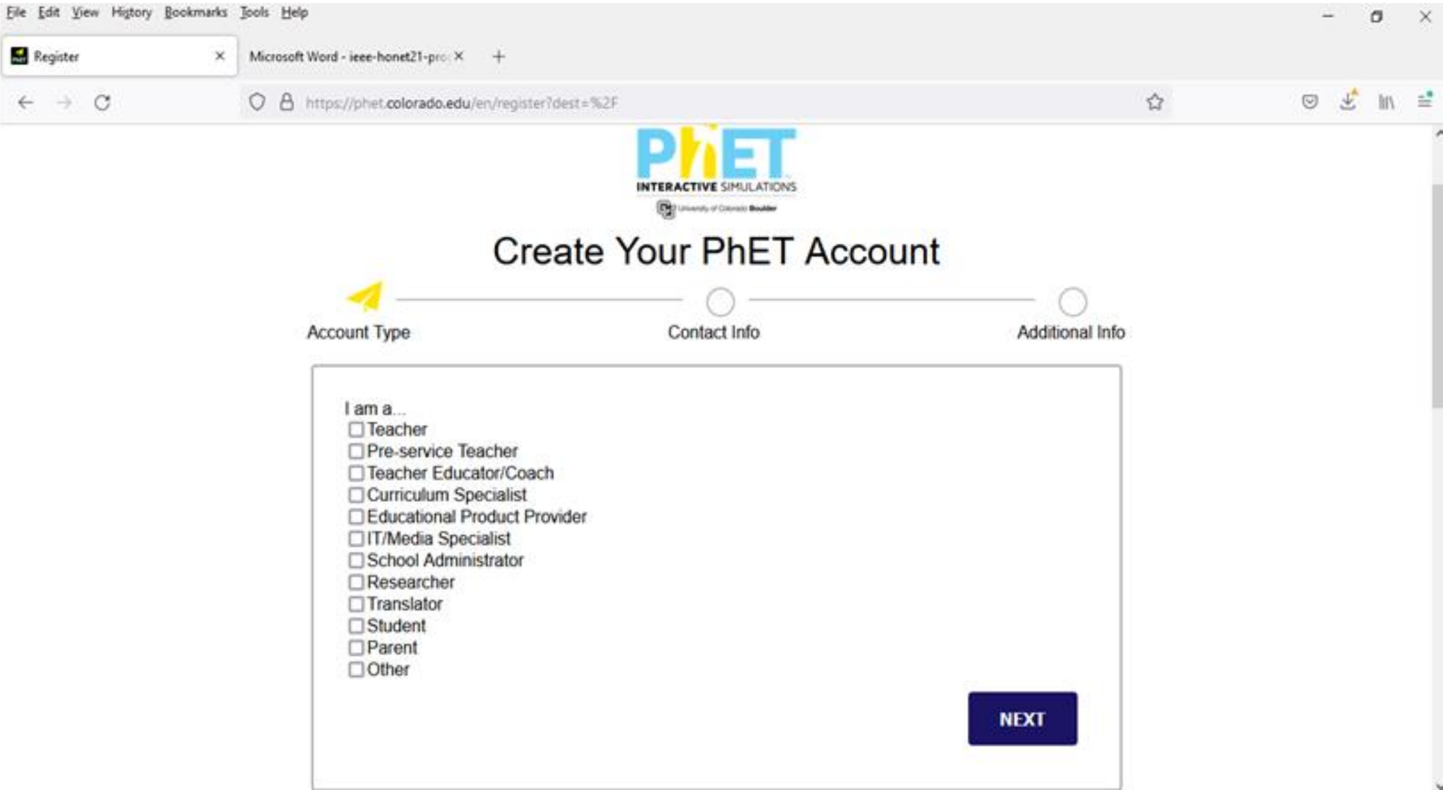


PhET Interactive Simulations

University of Colorado

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

https://phet.colorado.edu/



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.
-

Tips for Using PhET

PhET simulations are very flexible tools that can be used in many ways. Here, you will find videos and resources for learning about effective ways of integrating PhET simulations into your class.

A Brief Introduction to PhET

An overview of the PhET Simulations

PhET Interactive Simulations: Accessibility Features

University of Colorado

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

https://phet.colorado.edu/

Accessible Simulations

▼ Accessibility Features

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

INTERACT
DISCOVER
LEARN

167	123	3619
interactive simulations	language translations	teacher-submitted lessons

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!

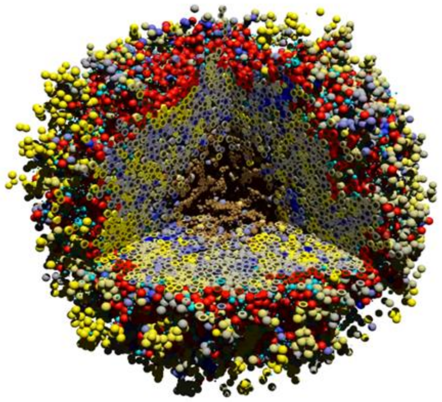
Friction

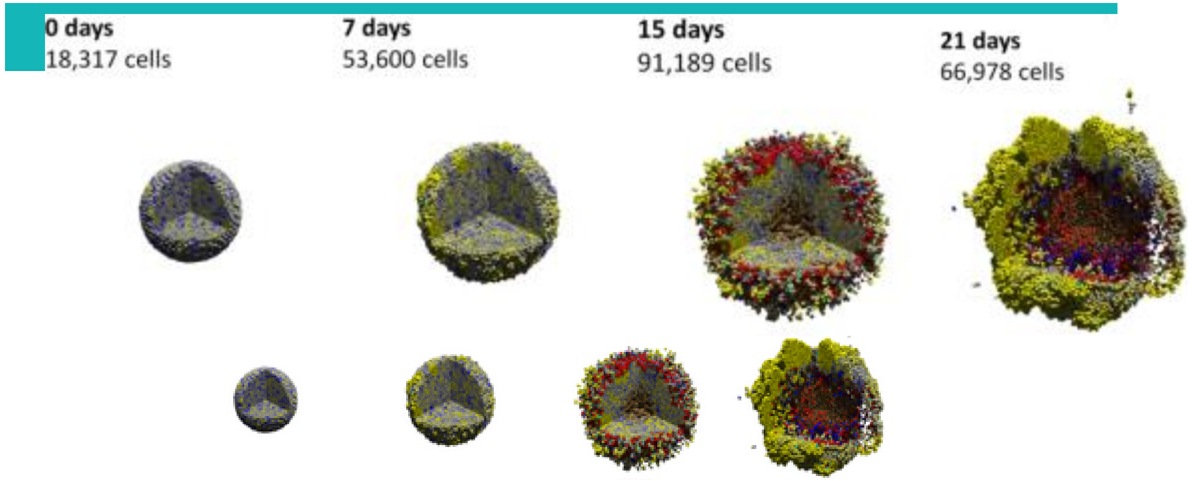
- Published Version: Friction

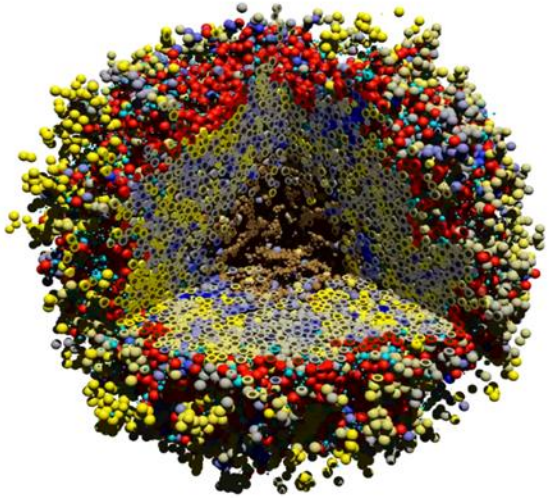
A complete list is available at: https://phet.colorado.edu/en/accessibility/prototypes

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

PhysiCell





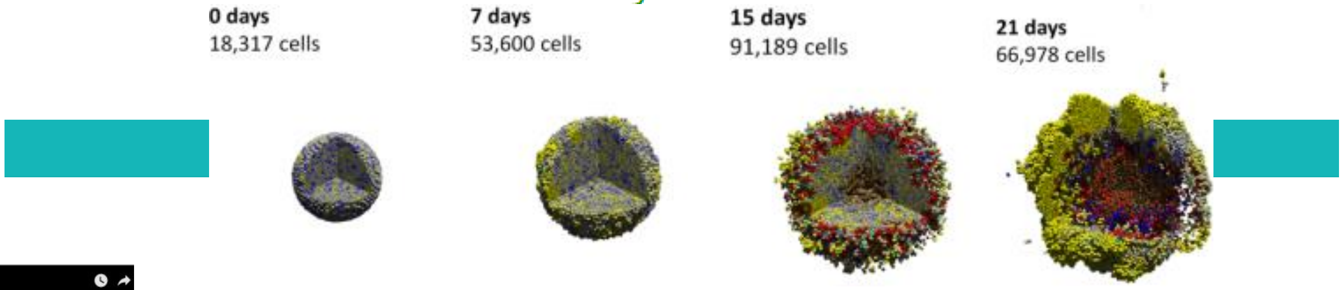


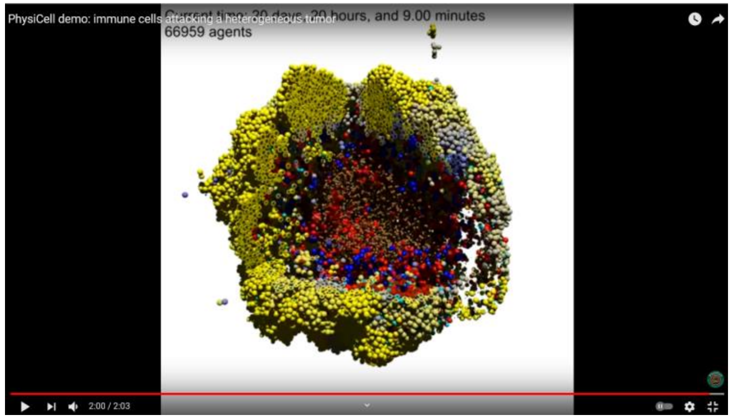
An open source physics-based cell simulator

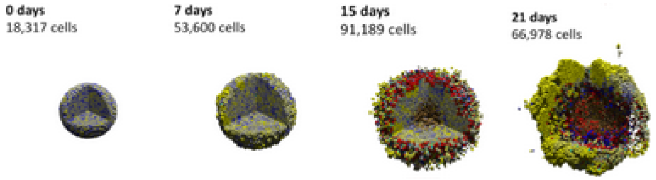
http://physicell.org/

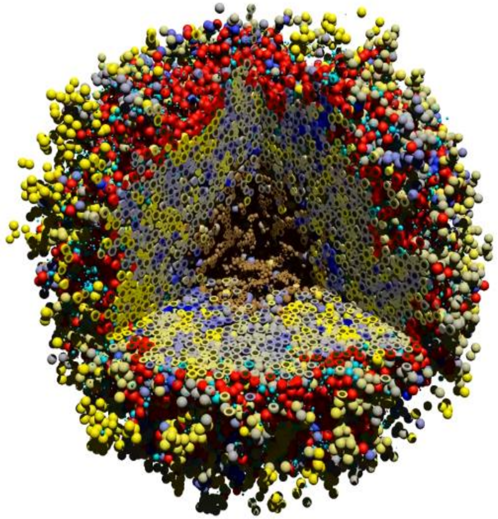
Physicell can also be accessed via nanoHub.

PhysiCell







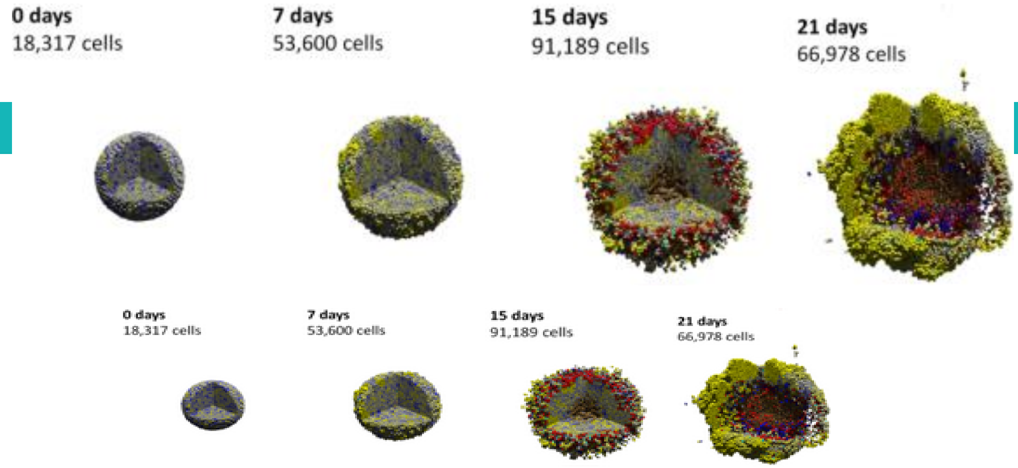


An open source physics-based cell simulator

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

https://youtu.be/nJ2urSm4ilU

PhysiCell



An open source physics-based cell simulator

http://physicell.org/

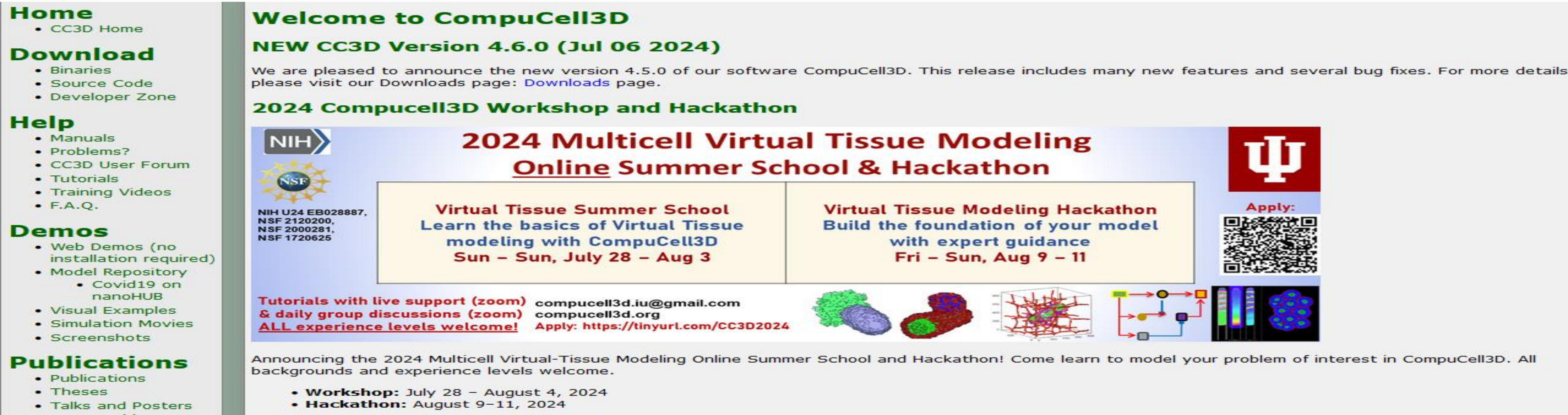
Physicell can also be accessed via nanoHub.

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).

CompuCell3D: https://compucell3d.org/

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.

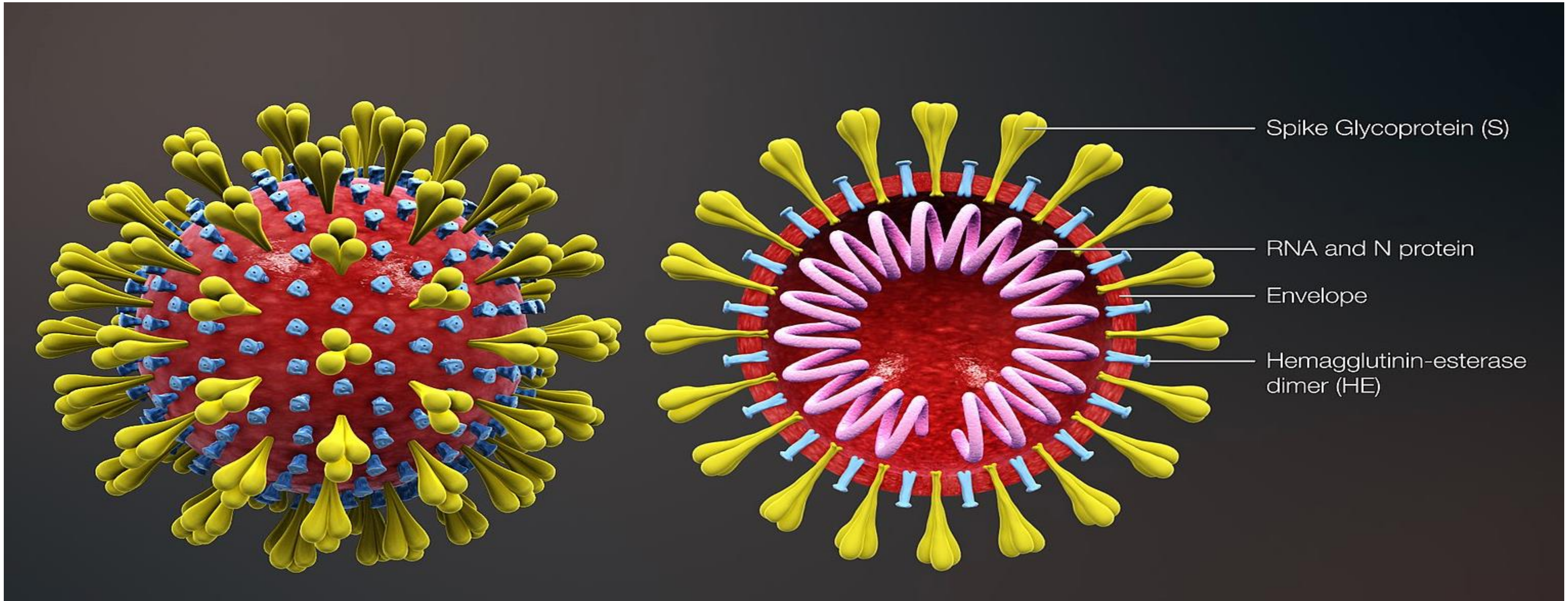


Example of the Application of CompuCell3D

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



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

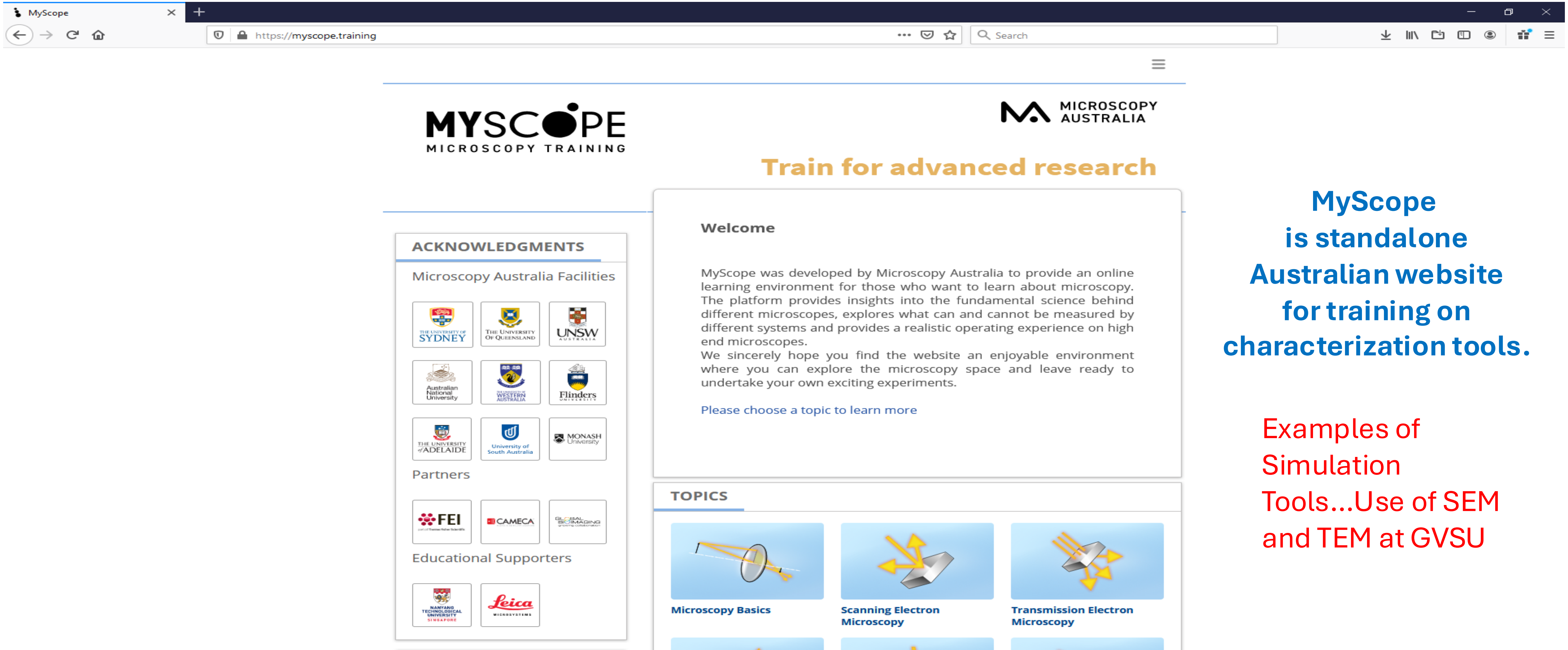
https://www.youtube.com/watch?v=edL8yHE8cO8&feature=youtu.be

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.

A great characterization virtual experience: MYSCOPE

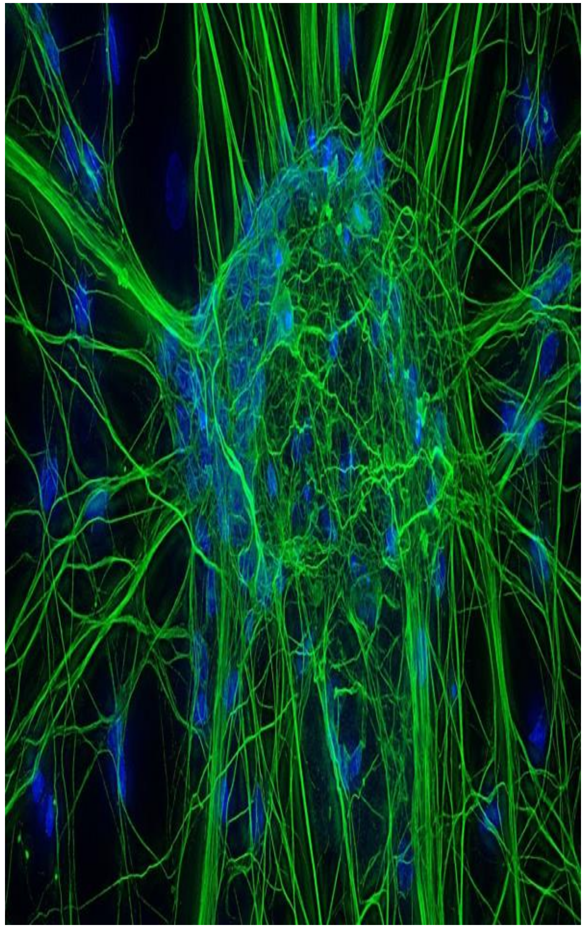


MyScope is standalone Australian website for training on characterization tools.

Examples of Simulation Tools…Use of SEM and TEM at GVSU

Need For Visualization at the Nanoscale

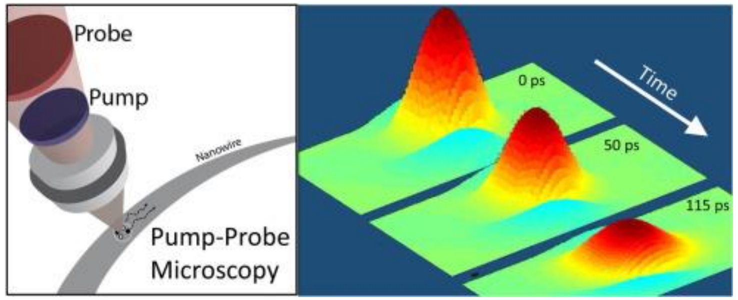
- Visualization of physical phenomena can confirm hypothesis
- Observation provides opportunities for the sample study without damaging .
- Objects under study may be too small for our hands to handle or manipulate
- Our students are motivated by "seeing for themselves"!
- Measurement tools for nanotechnology 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 & measurement at the nanoscale.



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

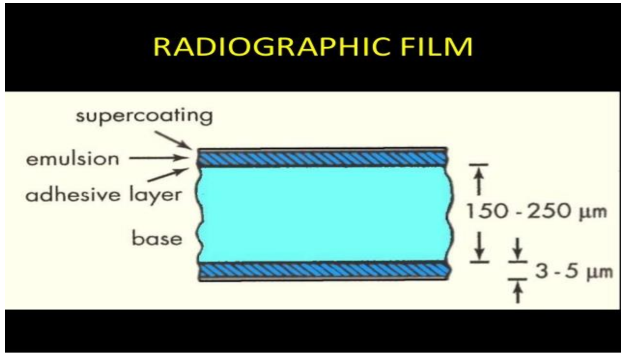
Advantages of Visualization at the Nanoscale

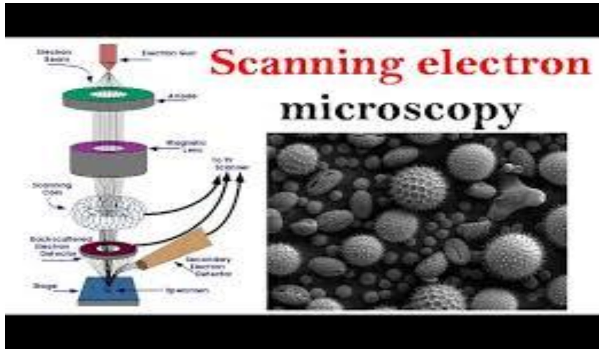
- Enhance students understanding of the properties of matter at the nanoscale which differ from bulk material.
- Help instructors improve teaching of abstract concepts of nanoscale phenomena.
- Understand the benefits and application of visualization at the nanoscale.
- Increase knowledge in the field 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**

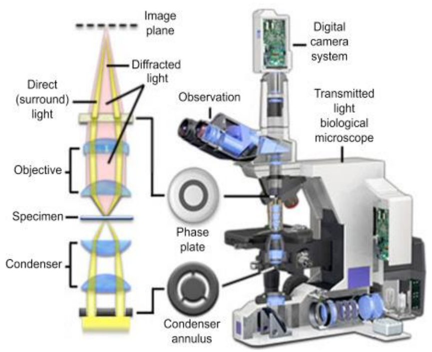
  Suffers from diffraction effect on sample surfaces.
  Limited resolution at nanoscale.

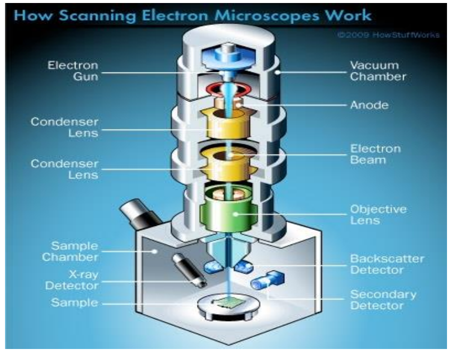
- **Scanning electron microscope (SEM)**

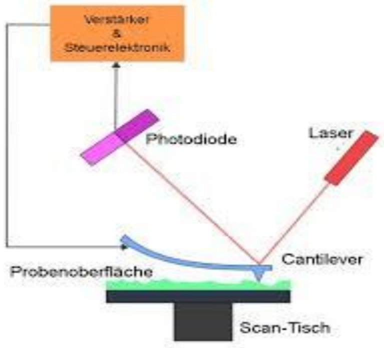
  Require the use of electron beams at high vacuum environment and cannot be used for biological non-conductive samples and samples under liquid.

- **Atomic Force Microscopy (AFM)**

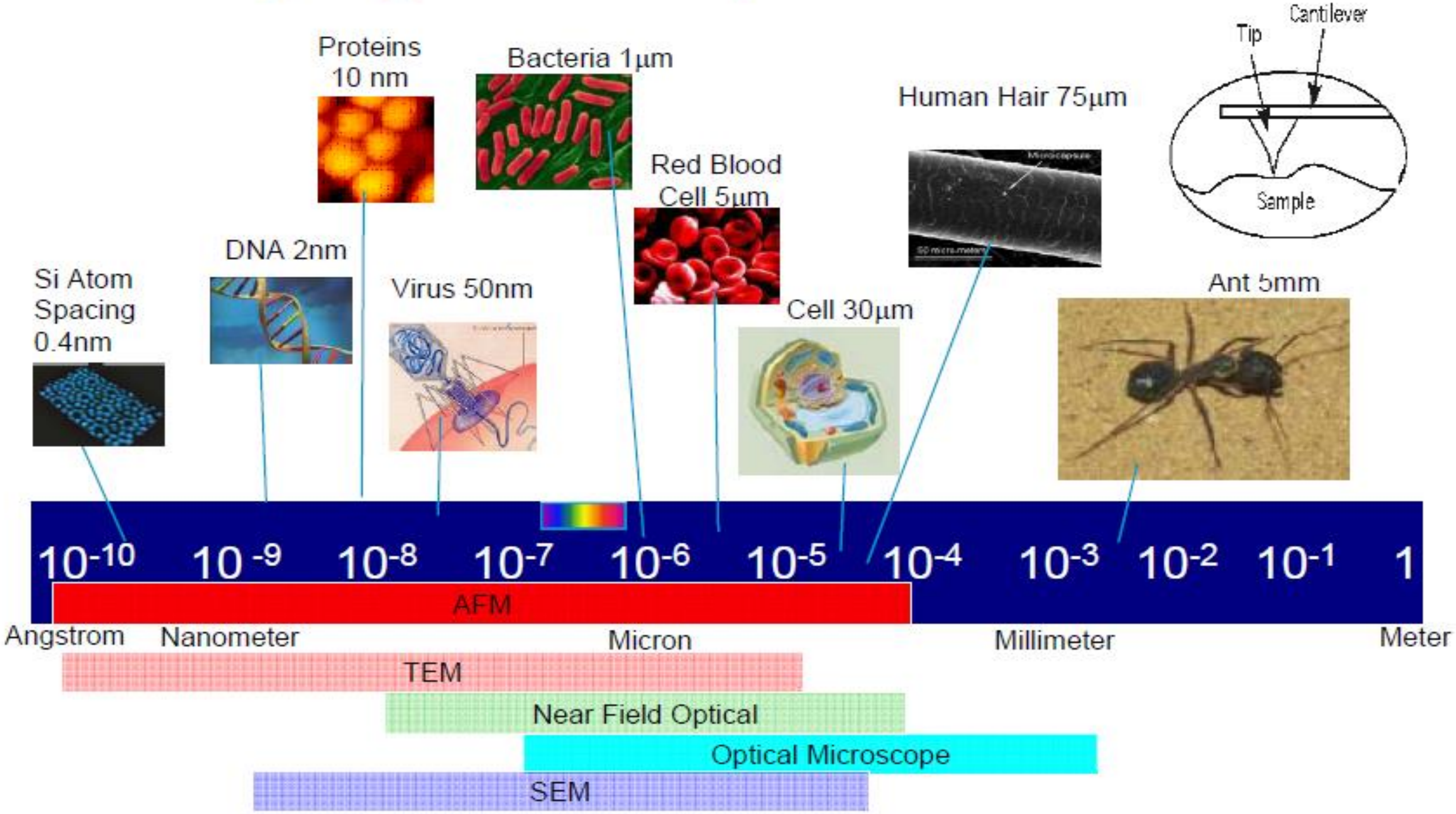
  Uses sharp probe scanning over the sample while maintaining a very close spacing to the surface . A tool to measure both topography and force-related material properties at the nanoscale.





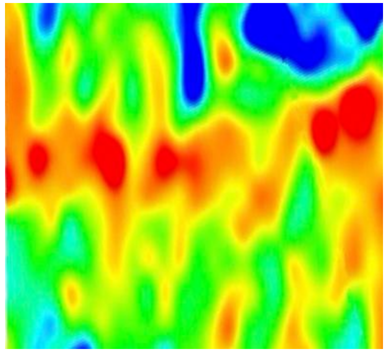


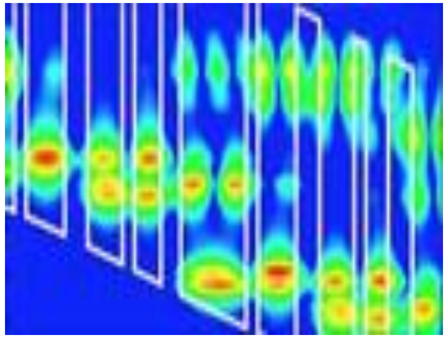
Imaging Techniques: Scales

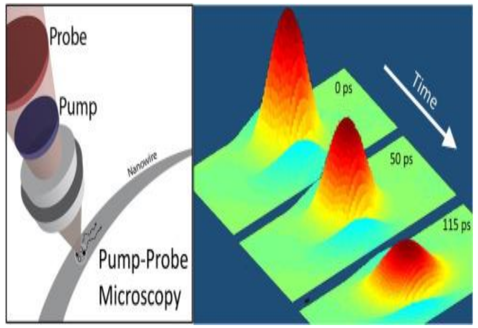


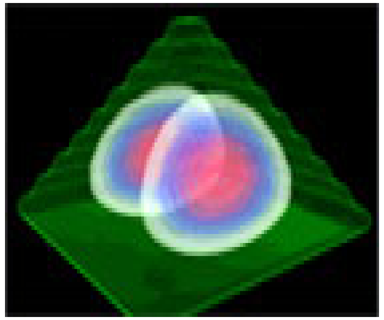
Visualization at the Nanoscale

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









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

REMOTE ACCESS INSTRUMENTS FOR NANOTECHNOLOGY
RAIN

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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Home | Educators | Remote Access

Getting Started | 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.

Mission Statement

https://youtu.be/Tz1AvCUqoNo

RAIN Network Partner Locations

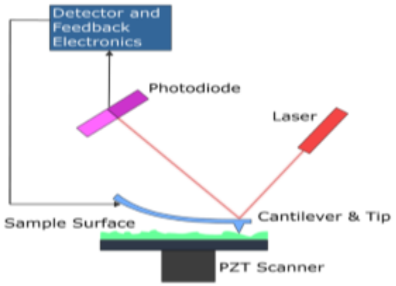
Learning through Visualization at the Nanoscale

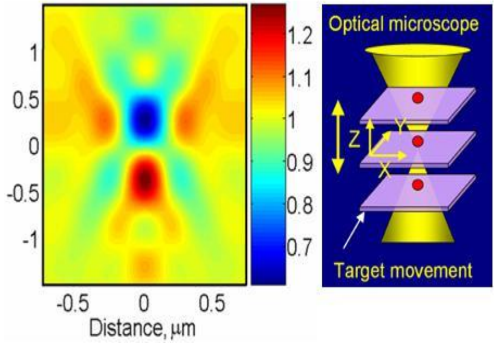
Types of Tools at RAIN

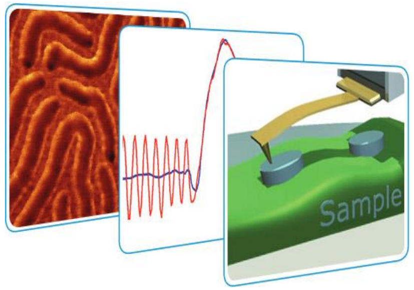
- RAIN allows students to access and control microscopes and analytical tools, to look at nanosized materials from the ease of classrooms, or home computers, across the country.
- Students control the tools over the Internet from 26 centers in real-time.

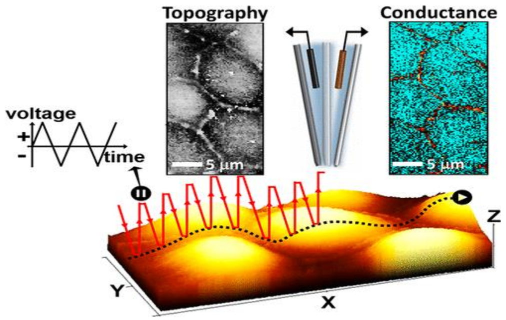
.

- 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









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

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 easyScan 2)

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

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.

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:

- Webcam
- Microphone
- Speakers
- 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

- This is where you will have live remote access to the lab equipment.
- 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.

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Web-Based Simulation and Remote Access Visualization Tools for Engineering and Technology Curricula

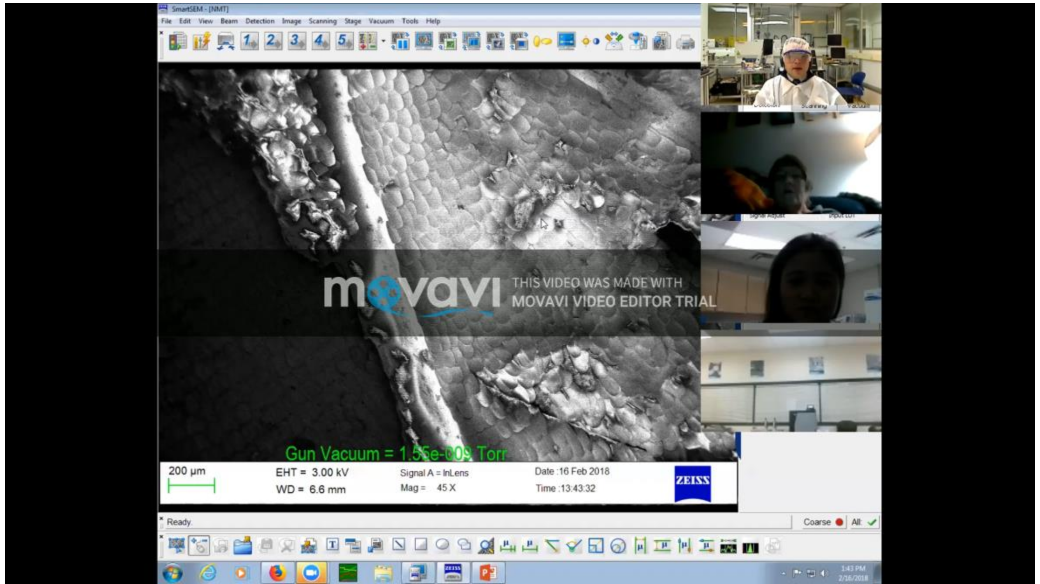
July 31, 2024

Dr. Ahmed S. Khan
Fulbright Specialist Scholar
Ex. Dean of the College of Engineering & Information Sciences
DeVry University, Addison, IL
Dr.a.s.khan@ieee.org

Use of Online Simulation Tools (SEM & TEM) at GVSU

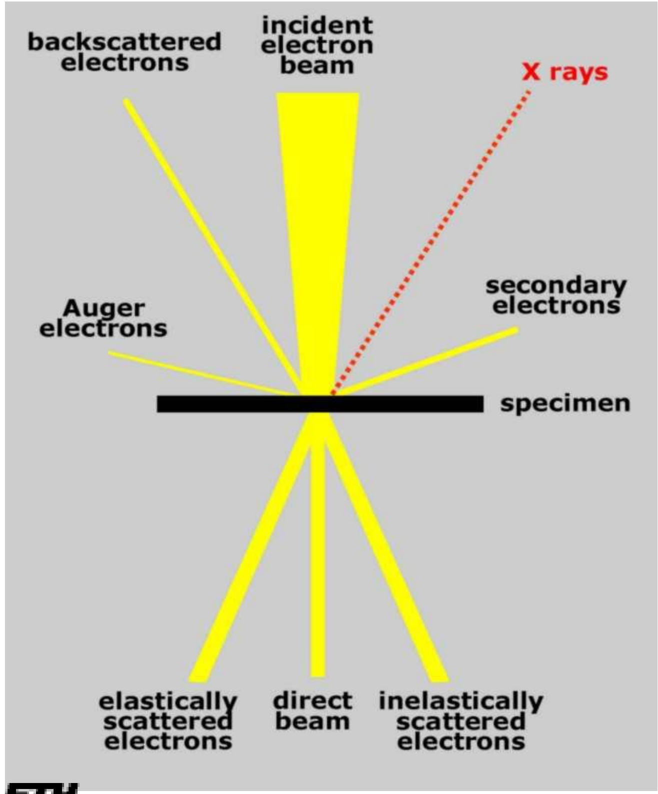
Dr. Atilla Ozgur Cakmak
Assistant Professor of Electrical Engineering
School of Engineering, Seymour and
Esther Padnos College of Engineering and Computing
Grand Valley State University
Allendale, MI
cakmaka@gvsu.edu
Dr. Sala Qazi
qazi@sunypoly.edu

- Scanning Electron Microscopy (SEM)
  - A very engaging tool for the students including K-12
  - Microscopy in general captivates general public interest since 1600s.
  - An expensive tool if Field Emission (FE)-SEM is desired



• Scanning Electron Microscopy (SEM) fundamentals

- One way to see things at the nano-scale is to use **beams of electrons**. These beams can be used to let us see size, shape, structure and even composition.
- When a beam of electrons hits a material (specimen), a number of responses occur. Some of the electrons may go through the specimen (transmitted electrons). Some may bounce back (backscattered electrons) and new electrons may be knocked off the atoms of the specimen and come back (secondary electrons and Auger electrons). In addition, photons, including high energy photons (x-rays), generated by the relaxing of excited atoms may come back.
- Each one of these responses can be exploited to "see" the specimen
- Seeing by using the backscattered and secondary electrons is called **scanning electron microscopy** (SEM). It is called **field emission scanning electron microscopy** (FE-SEM) when the impinging beam of electrons is produced by quantum mechanical tunneling.



ETH

Image Credits:
http://www.microscopy.ethz.ch/interactions.htm

- **<u>Vacuum</u>**- necessary for tool operation; column (high), chamber (low)
- **<u>Electron gun</u>**- source of the electron beam
- **<u>Condenser Lenses</u>** – focus and reduce/expand beam
- **<u>Aperture</u>**- series of micron-scale holes in metal film which block outer parts of beam
- **<u>Gun valve</u>**- pressure valve separating gun and sample chambers
- **<u>Objective lens</u>**- focuses electron beam on specimen surface
- **<u>Deflector Coils</u>**- create scan pattern and beam raster pattern
- **<u>Specimen position</u>**- x,y,z, tilt, and rotation on goniometric stage

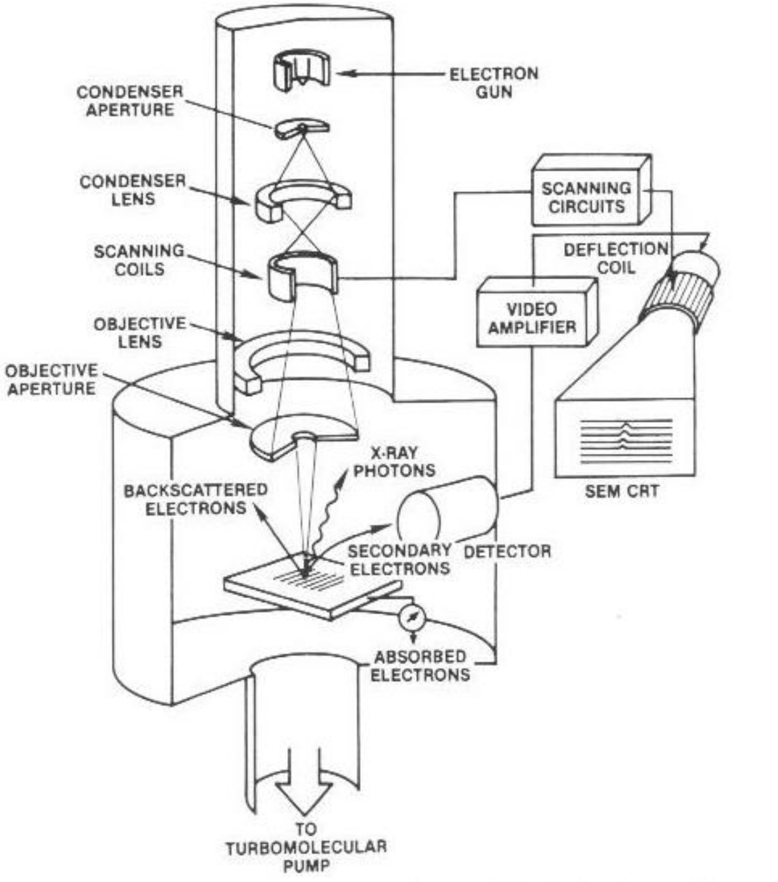
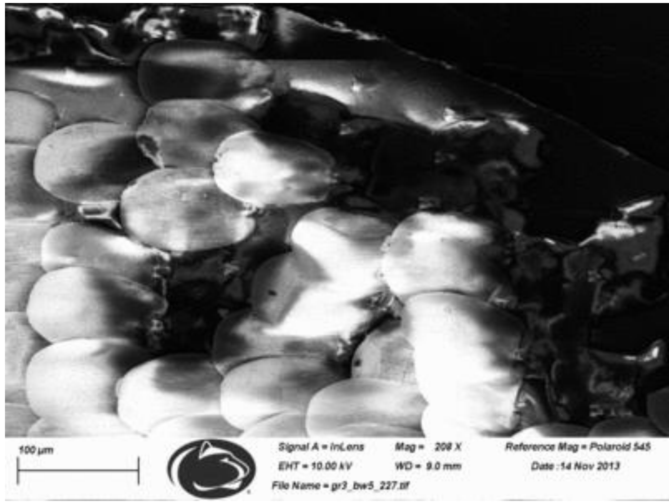


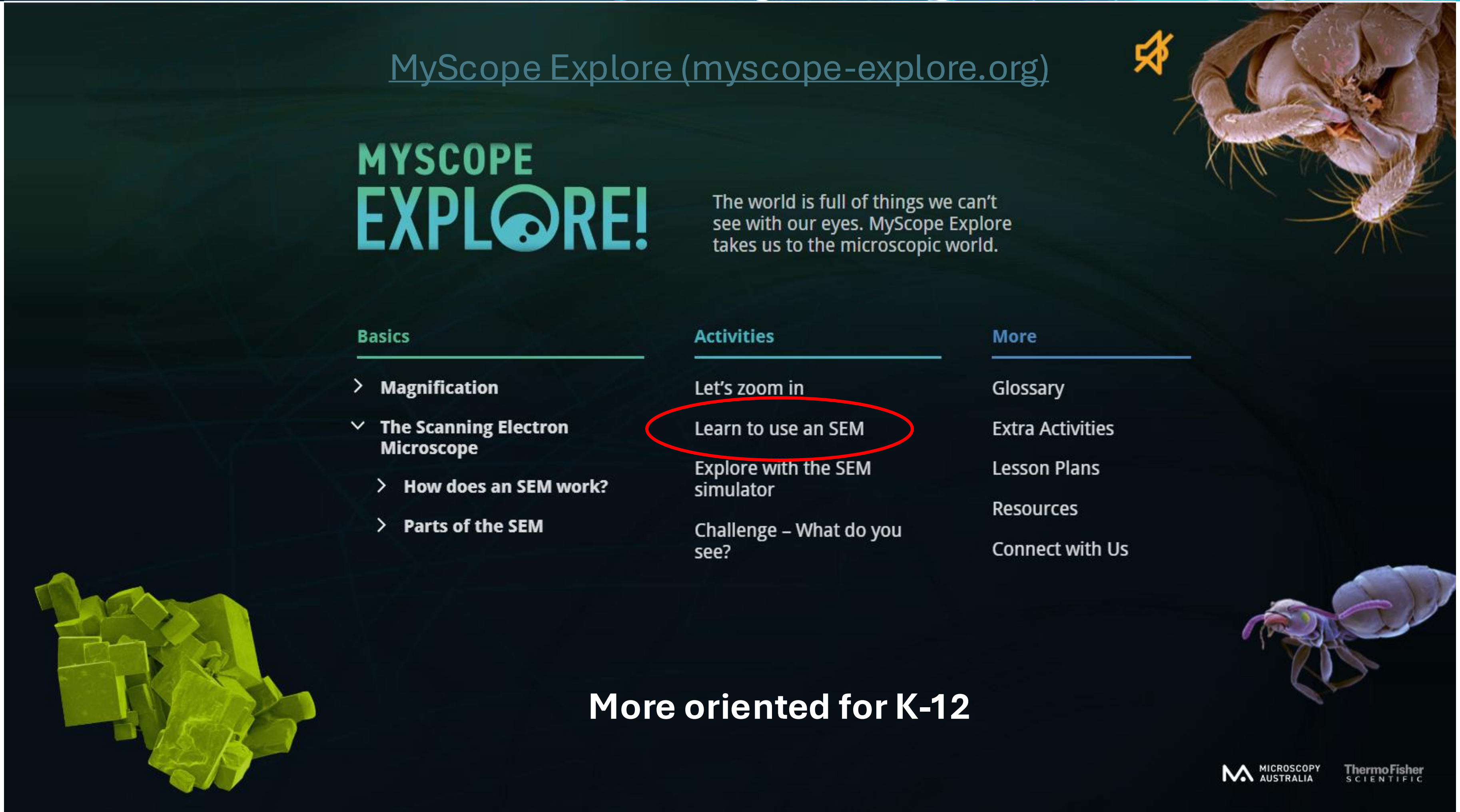
Image Credits: Semiconductor Material and Device Characterization, 2nd ed. Dieter K. Schroder, John Wiley & Sons, Inc.

X, Y Coordinate	Time (µSec.)
1, 10	0:01
2, 10	0:38
3, 10	1:15
4, 10	1:52
5, 10	2:29
6, 10	3:06
7, 10	3:43
8, 10	4:20
9, 10	4:57
10, 10	5:04
11, 10	5:11
12, 10	5:18

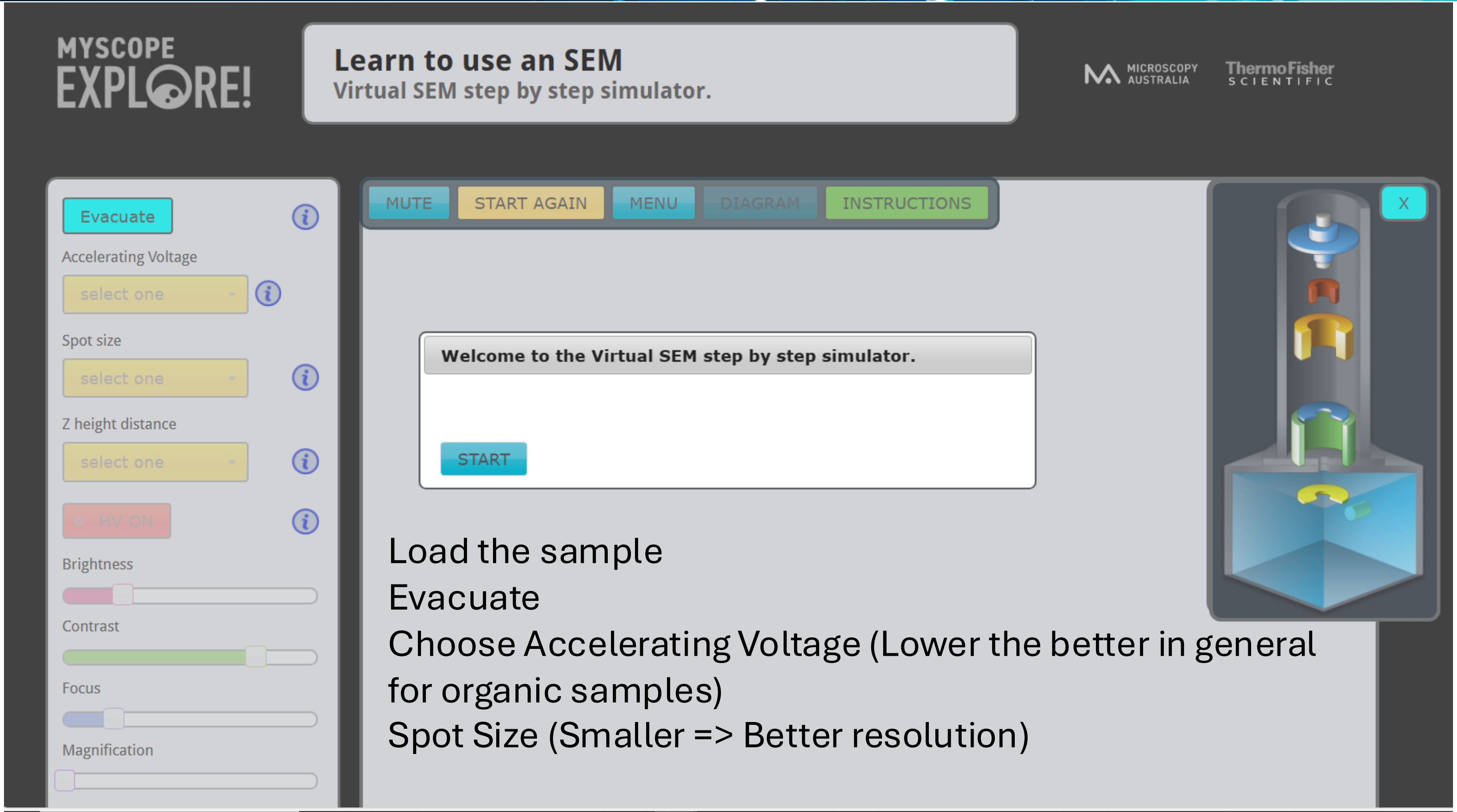
Time	Signal Intensity
0:01	■□□□□□□□
0:38	■□□□□□□□
1:15	■■■■□□□□
1:52	■■■■■■■□
2:29	■□□□□□□□
3:06	■■■■■■■□
3:43	■■■■■■■□
4:20	■□□□□□□□
4:57	■■■■■■■□
5:04	■■■■□□□□
5:11	■□□□□□□□
5:18	■□□□□□□□

It’s me, Mario





More oriented for K-12

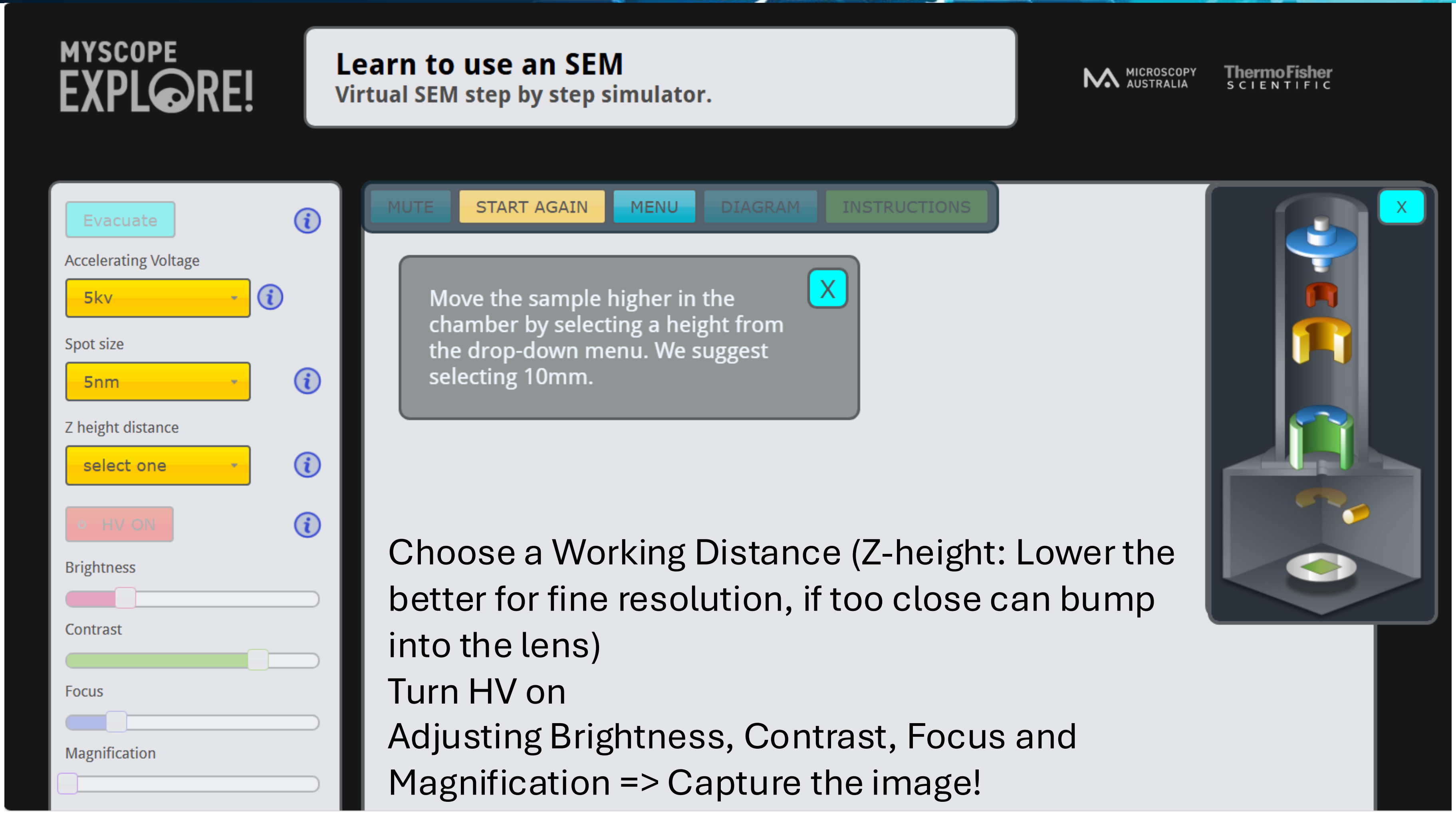


Load the sample

Evacuate

Choose Accelerating Voltage (Lower the better in general for organic samples)

Spot Size (Smaller => Better resolution)



Choose a Working Distance (Z-height: Lower the better for fine resolution, if too close can bump into the lens)

Turn HV on

Adjusting Brightness, Contrast, Focus and Magnification => Capture the image!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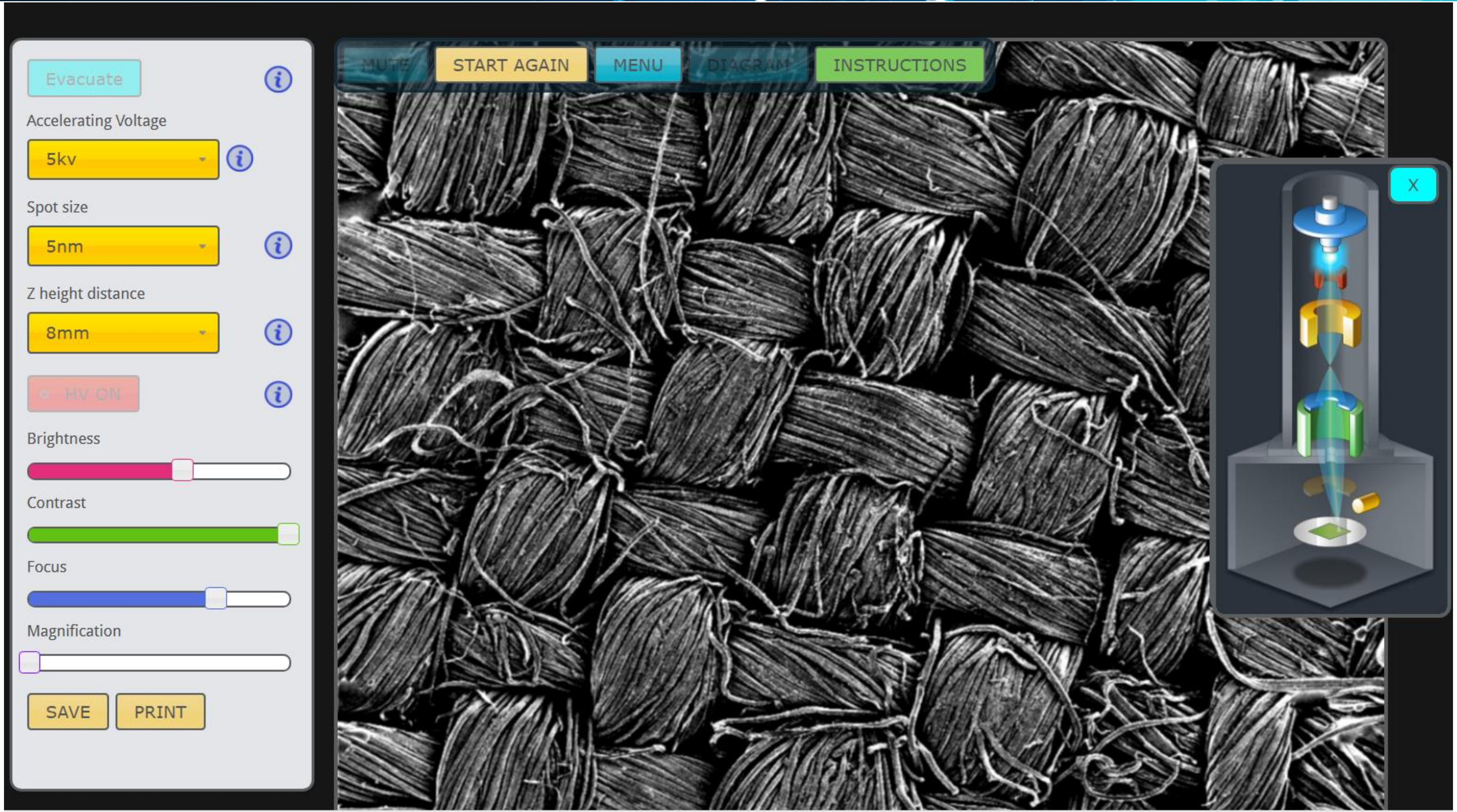
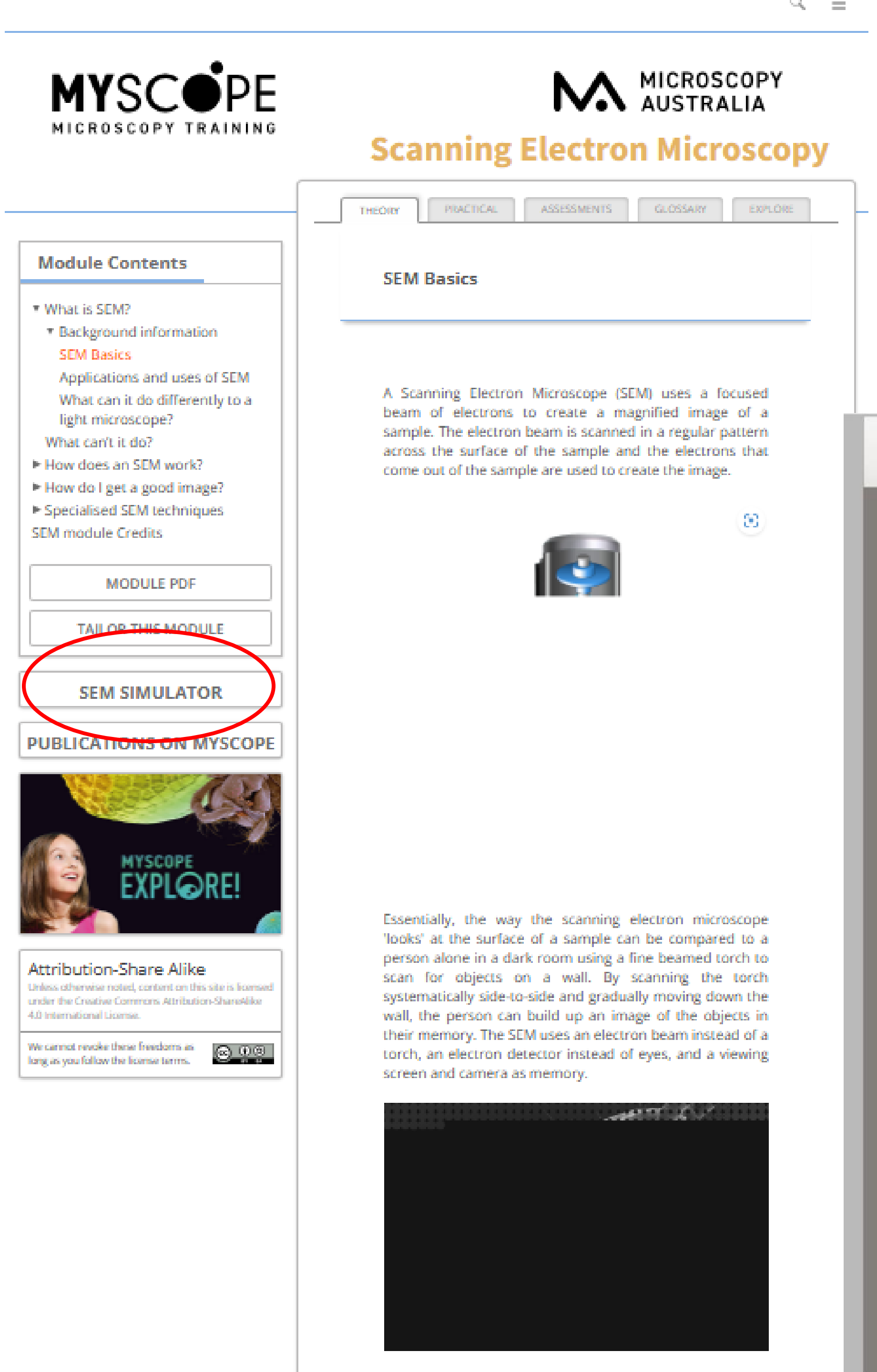

Evacuate
Accelerating Voltage
5kv
Spot size
5nm
Z height distance
8mm
HV ON
Brightness
Contrast
Focus
Magnification
SAVE
PRINT
MUTE
START AGAIN
MENU
DIAGRAM
INSTRUCTIONS
X

[MyScope - Train for advanced research]

There are several excellent simulators for TC and CC students as well as higher level training for instructors.

Going to quickly show some snapshots from SEM, EDS, TEM, FIB and SPM


MYSCOPE
MICROSCOPY TRAINING
MICROSCOPY AUSTRALIA
Scanning Electron Microscopy
THEORY
PRACTICAL
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EXPLORE
Module Contents
What is SEM?
Background information
SEM Basics
Applications and uses of SEM
What can it do differently to a light microscope?
What can't it do?
How does an SEM work?
How do I get a good image?
Specialised SEM techniques
SEM module Credits
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SEM SIMULATOR
PUBLICATIONS ON MYSCOPE
MYSCOPE EXPLORE!
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SEM Basics
A Scanning Electron Microscope (SEM) uses a focused beam of electrons to create a magnified image of a sample. The electron beam is scanned in a regular pattern across the surface of the sample and the electrons that come out of the sample are used to create the image.
Essentially, the way the scanning electron microscope 'looks' at the surface of a sample can be compared to a person alone in a dark room using a fine beamed torch to scan for objects on a wall. By scanning the torch systematically side-to-side and gradually moving down the wall, the person can build up an image of the objects in their memory. The SEM uses an electron beam instead of a torch, an electron detector instead of eyes, and a viewing screen and camera as memory.


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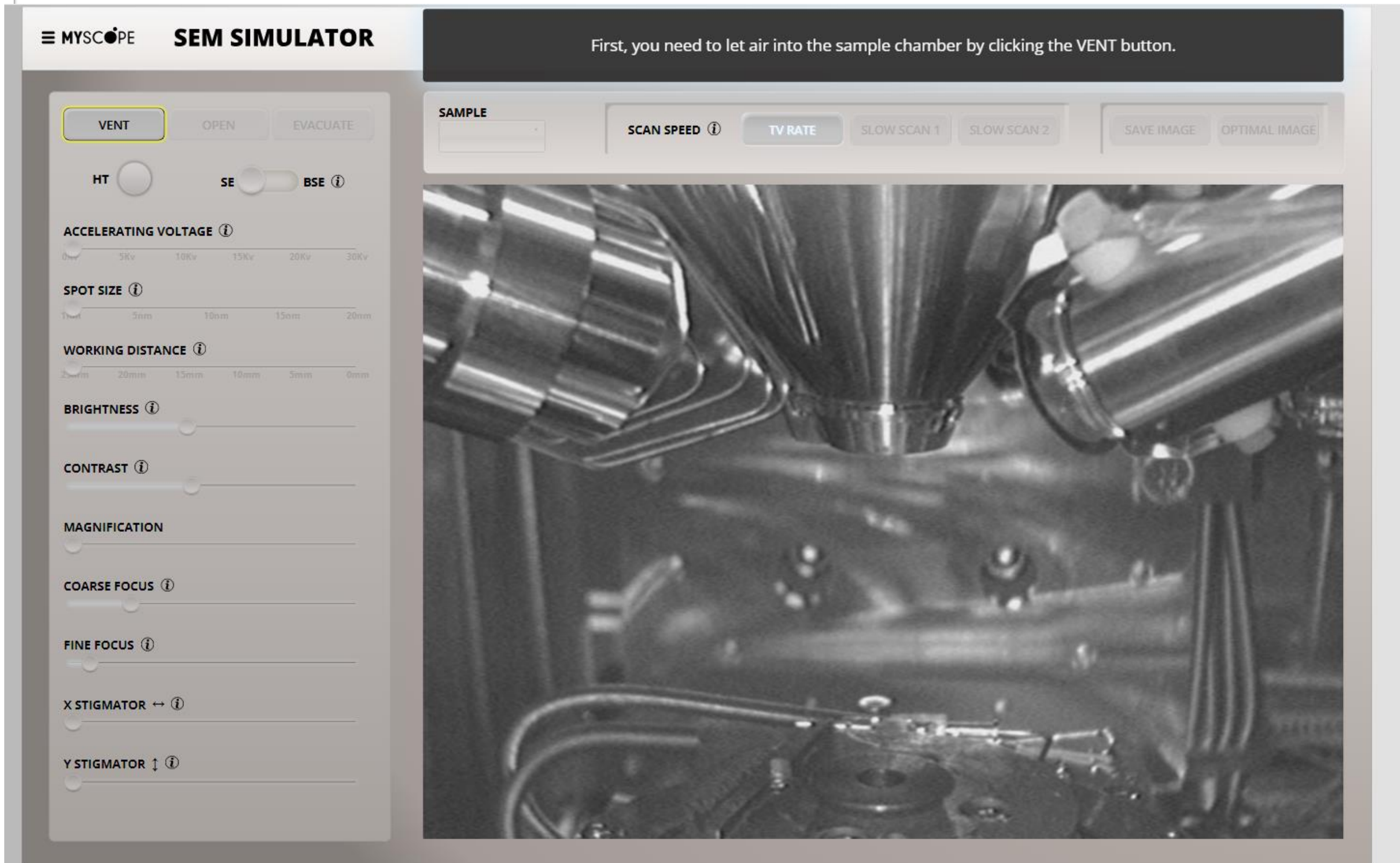
MYSCOPE
SEM SIMULATOR
First, you need to let air into the sample chamber by clicking the VENT button.
VENT
OPEN
EVACUATE
HT
SE
BSE
ACCELERATING VOLTAGE
SPOT SIZE
WORKING DISTANCE
BRIGHTNESS
CONTRAST
MAGNIFICATION
COARSE FOCUS
FINE FOCUS
X STIGMATOR ↔
Y STIGMATOR ↕
SAMPLE
SCAN SPEED
TV RATE
SLOW SCAN 1
SLOW SCAN 2
SAVE IMAGE
OPTIMAL IMAGE


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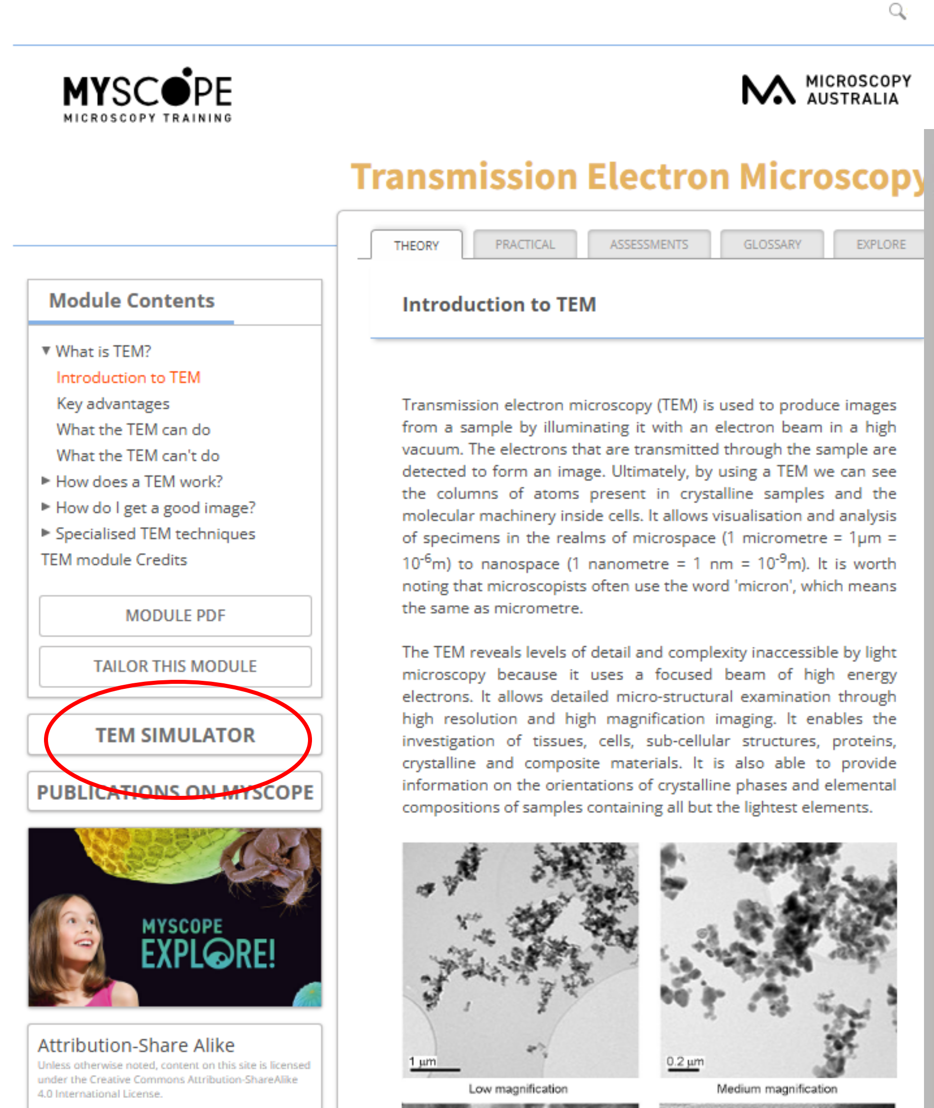
MYSCOPE
MICROSCOPY TRAINING
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Transmission Electron Microscopy
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What the TEM can't do
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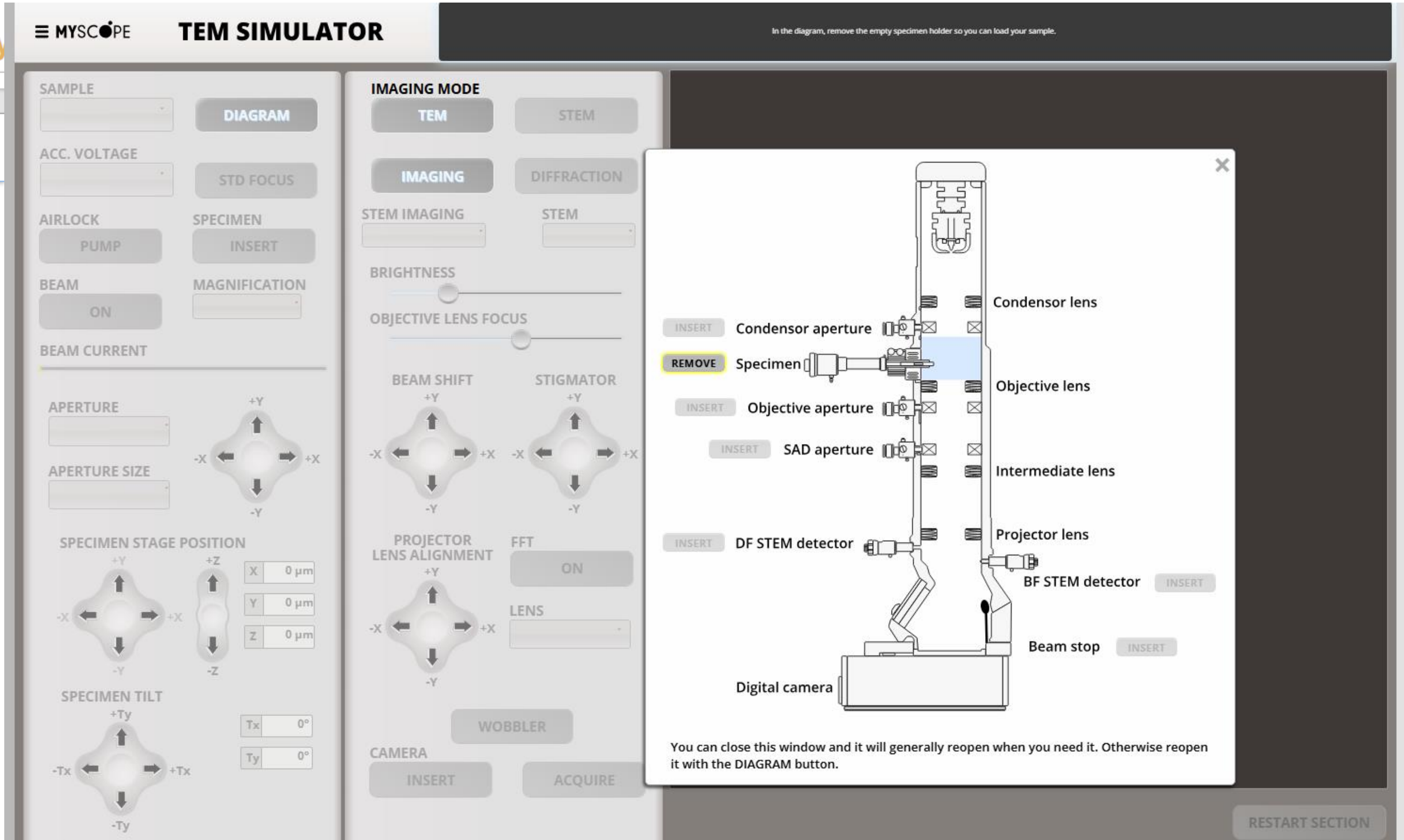
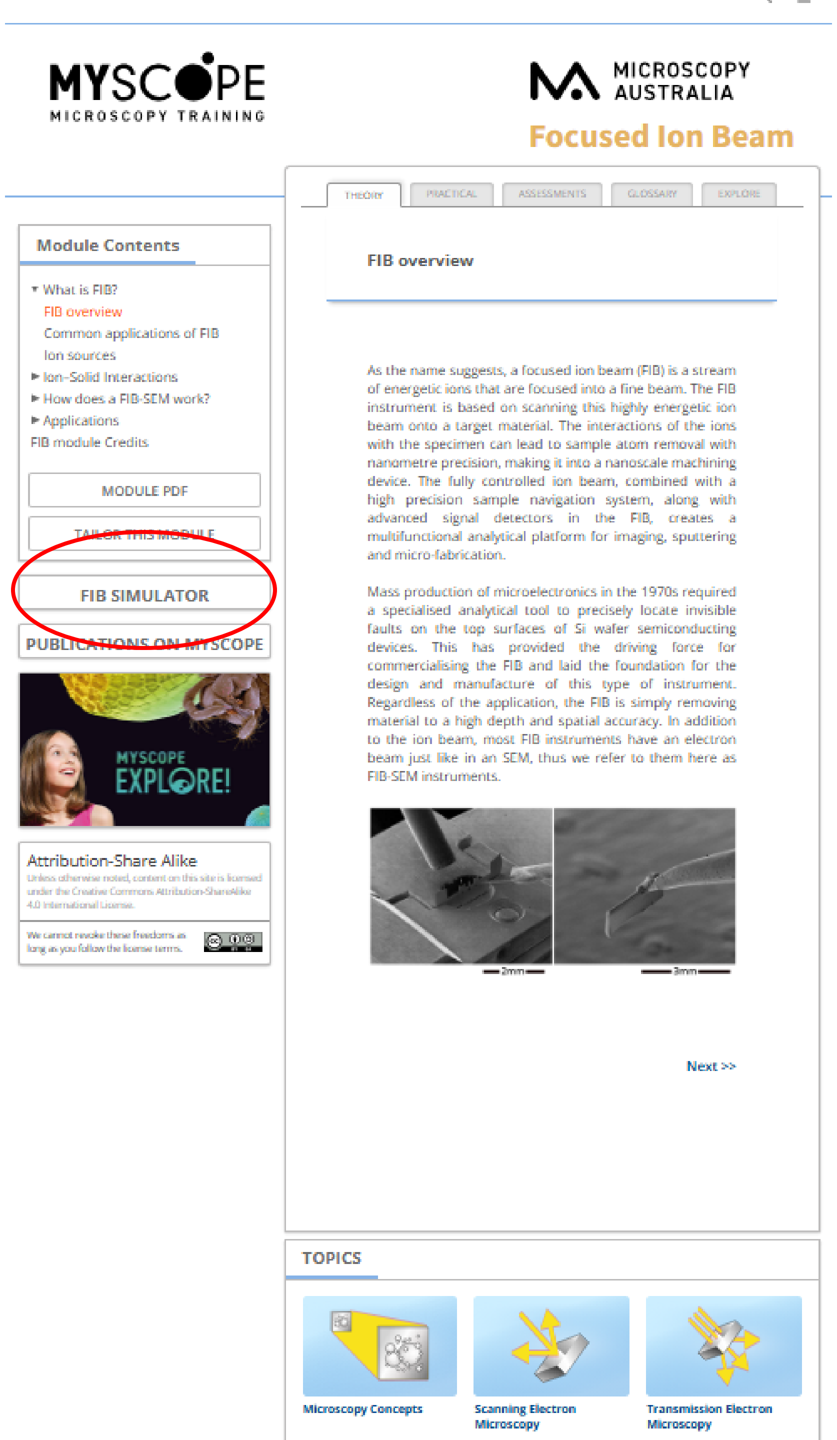
Introduction to TEM
Transmission electron microscopy (TEM) is used to produce images from a sample by illuminating it with an electron beam in a high vacuum. The electrons that are transmitted through the sample are detected to form an image. Ultimately, by using a TEM we can see the columns of atoms present in crystalline samples and the molecular machinery inside cells. It allows visualisation and analysis of specimens in the realms of microspace (1 micrometre = 1μm = 10^{-6}m) to nanospace (1 nanometre = 1 nm = 10^{-9}m). It is worth noting that microscopists often use the word 'micron', which means the same as micrometre.
The TEM reveals levels of detail and complexity inaccessible by light microscopy because it uses a focused beam of high energy electrons. It allows detailed micro-structural examination through high resolution and high magnification imaging. It enables the investigation of tissues, cells, sub-cellular structures, proteins, crystalline and composite materials. It is also able to provide information on the orientations of crystalline phases and elemental compositions of samples containing all but the lightest elements.
1 μm
Low magnification
0.2 μm
Medium magnification


MYSCOPE
TEM SIMULATOR
In the diagram, remove the empty specimen holder so you can load your sample.
SAMPLE
DIAGRAM
ACC. VOLTAGE
STD FOCUS
AIRLOCK
PUMP
SPECIMEN
INSERT
BEAM
ON
MAGNIFICATION
BEAM CURRENT
APERTURE
APERTURE SIZE
SPECIMEN STAGE POSITION
SPECIMEN TILT
IMAGING MODE
TEM
STEM
IMAGING
DIFFRACTION
STEM IMAGING
BRIGHTNESS
OBJECTIVE LENS FOCUS
BEAM SHIFT
STIGMATOR
PROJECTOR LENS ALIGNMENT
FFT
LENS
WOBBLER
CAMERA
INSERT
ACQUIRE
Condensor lens
Condensor aperture
REMOVE
Specimen
Objective lens
Objective aperture
SAD aperture
Intermediate lens
Projector lens
DF STEM detector
BF STEM detector
Beam stop
Digital camera
You can close this window and it will generally reopen when you need it. Otherwise reopen it with the DIAGRAM button.
RESTART SECTION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MICROSCOPY AUSTRALIA
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Ion-Solid Interactions
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FIB overview
As the name suggests, a focused ion beam (FIB) is a stream of energetic ions that are focused into a fine beam. The FIB instrument is based on scanning this highly energetic ion beam onto a target material. The interactions of the ions with the specimen can lead to sample atom removal with nanometre precision, making it into a nanoscale machining device. The fully controlled ion beam, combined with a high precision sample navigation system, along with advanced signal detectors in the FIB, creates a multifunctional analytical platform for imaging, sputtering and micro-fabrication.
Mass production of microelectronics in the 1970s required a specialised analytical tool to precisely locate invisible faults on the top surfaces of Si wafer semiconducting devices. This has provided the driving force for commercialising the FIB and laid the foundation for the design and manufacture of this type of instrument. Regardless of the application, the FIB is simply removing material to a high depth and spatial accuracy. In addition to the ion beam, most FIB instruments have an electron beam just like in an SEM, thus we refer to them here as FIB-SEM instruments.
Next >>
TOPICS
Microscopy Concepts
Scanning Electron Microscopy
Transmission Electron Microscopy


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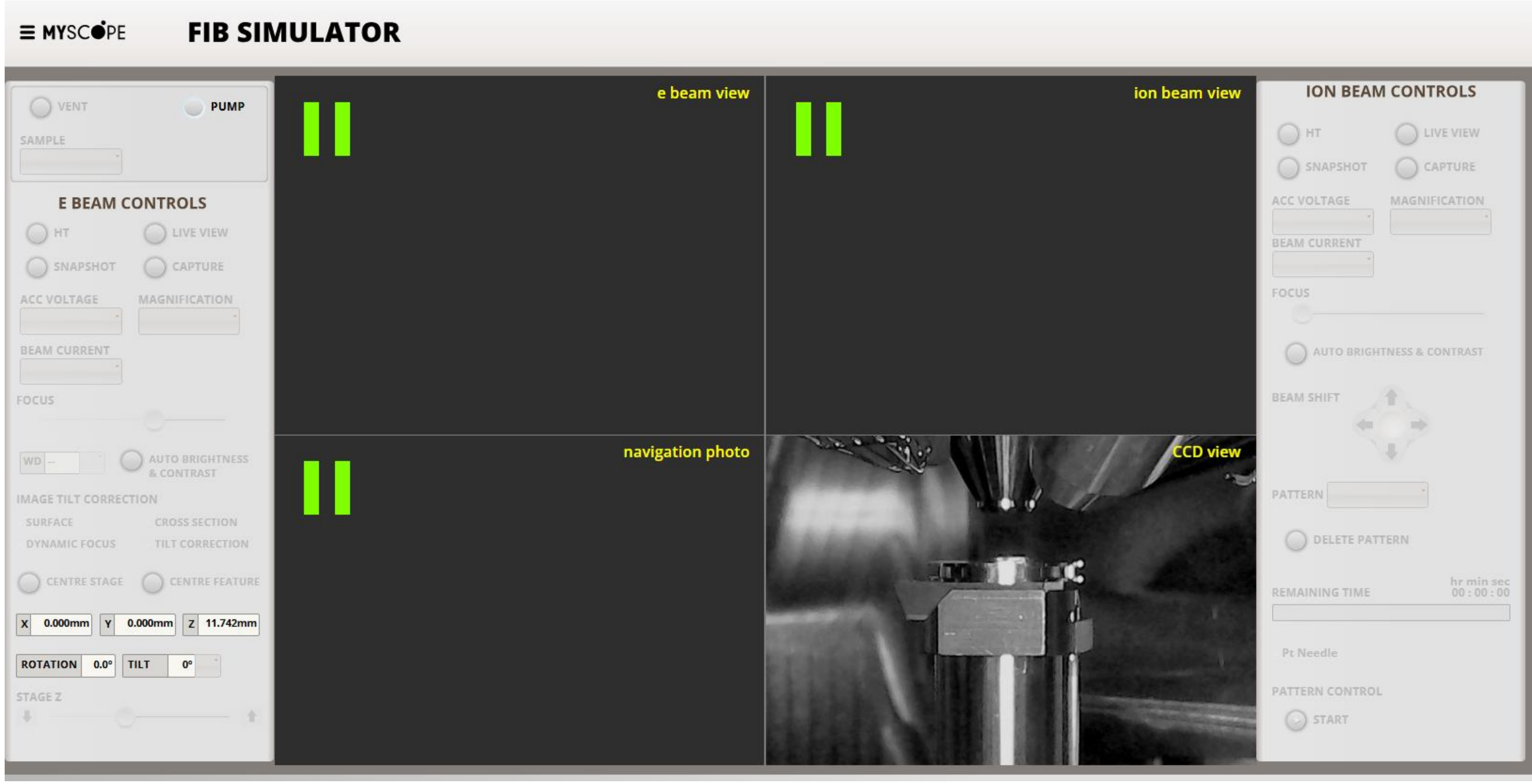
MYSCOPE
FIB SIMULATOR
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SNAPSHOT
CAPTURE
ACC VOLTAGE
MAGNIFICATION
BEAM CURRENT
FOCUS
AUTO BRIGHTNESS & CONTRAST
IMAGE TILT CORRECTION
SURFACE
CROSS SECTION
DYNAMIC FOCUS
TILT CORRECTION
CENTRE STAGE
CENTRE FEATURE
X 0.000mm
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ion beam view
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CCD view
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SNAPSHOT
CAPTURE
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MAGNIFICATION
BEAM CURRENT
FOCUS
AUTO BRIGHTNESS & CONTRAST
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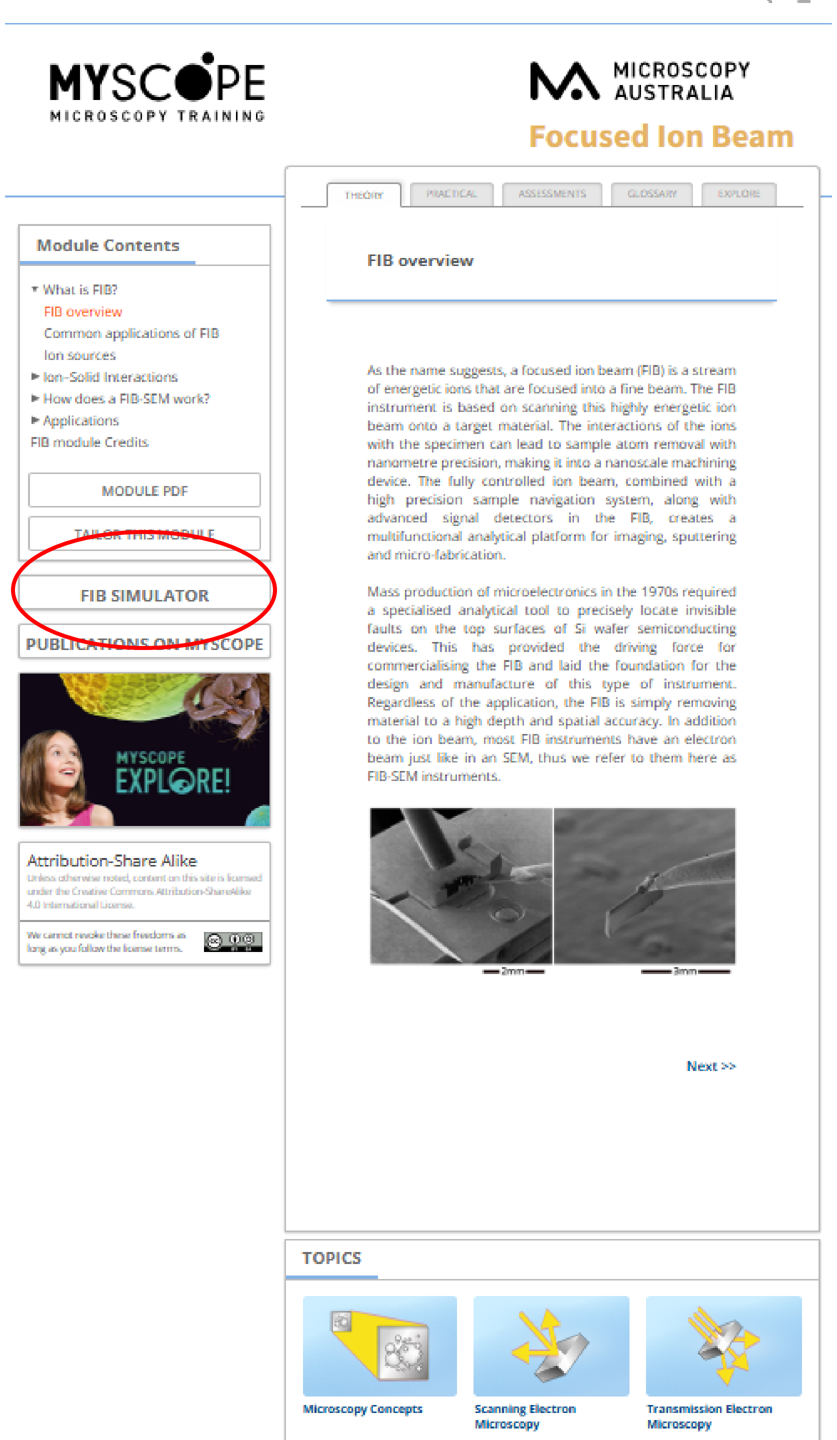
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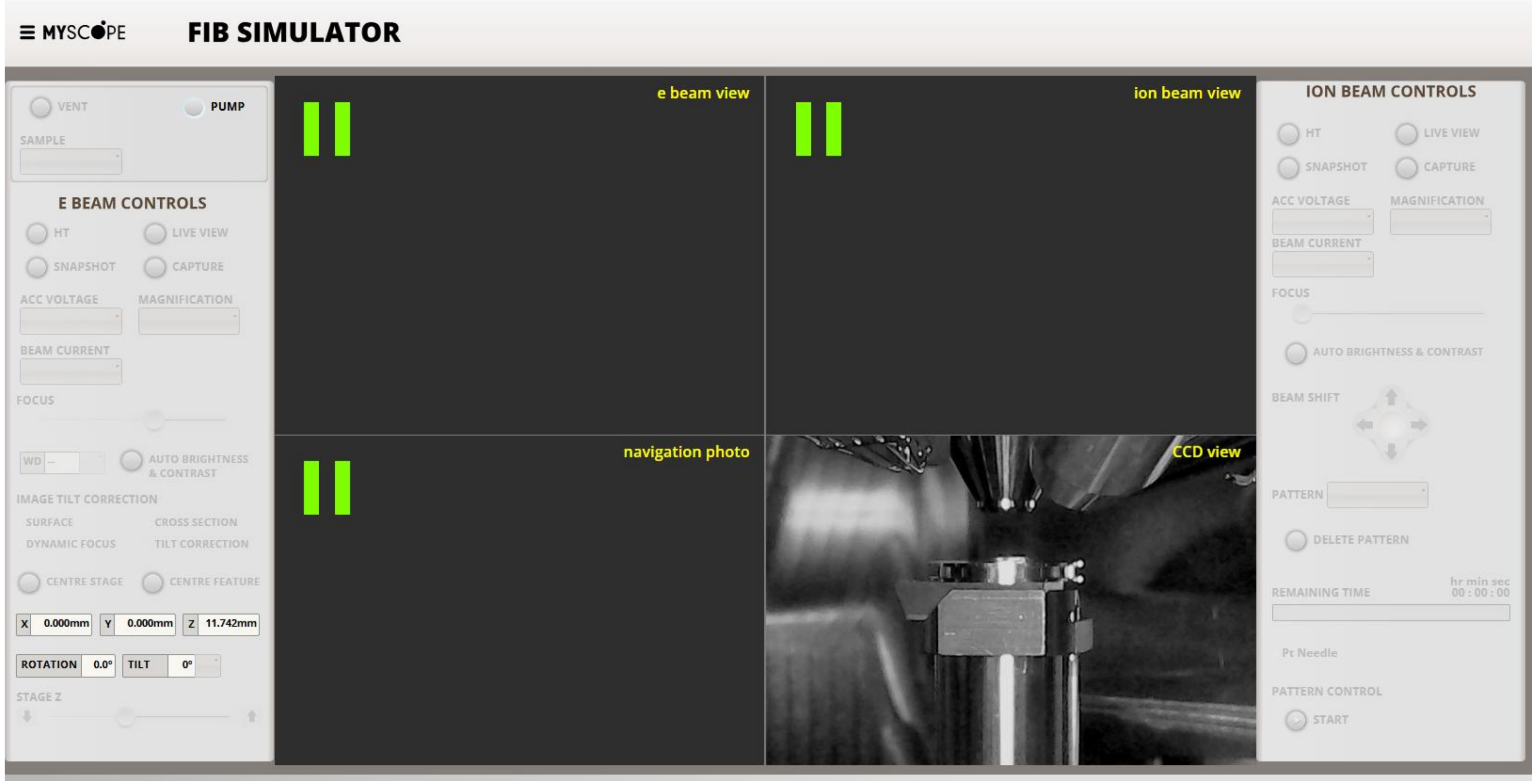
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CENTRE FEATURE
X 0.000mm
Y 0.000mm
Z 11.742mm
ROTATION 0.0°
TILT 0°
STAGE Z
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ion beam view
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PATTERN CONTROL
START

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.

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

Dr. Ahmed S. Khan

dr. a.s.khan@ieee.org

Dr. Atilla Ozgur Cakmak

cakmaka@gvsu.edu

Dr. Salahuddin Qazi

qazi@sunypoly.edu

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

Conclusion

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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.
10. MYSCOPE is an excellent online tool for incorporating topics like SEM, EDS, TEM, FIB and SPM into curricula.

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