HI-TEC 2020 TRANSFORMED

High Impact Technology Exchange Conference

JULY 29–30

MNT^{e}SIG MICRO NANO TECHNOLOGY education SPECIAL INTEREST GROUP

MNT Education Special Interest Group (MNT^{e}SIG Live) 2020 Virtual Conference Via Zoom, July 27-28, 2020

Online Visualization and Simulation Tools for Teaching Nanotechnology

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Online Visualization and Simulation Tools for Teaching Nanotechnology

Abstract

Visualization and Simulation enhance students' understanding of the material world at nanoscale. The purpose of presentation is to discuss the use of free online visualization and simulation tools for teaching Nanotechnology courses. Professors can use these online tools to enhance students learning of complex concepts at nanoscale without buying the expensive equipment. These tools include 26 RAIN (remote access instruments in nanotechnology) nodes for accessing visualization instruments and 500+ simulation tools at nanoHuB allowing students to simulate and understand nanotechnology concepts; and CompuCell3D, a 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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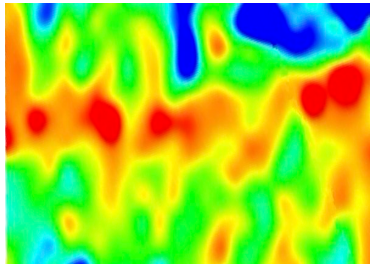
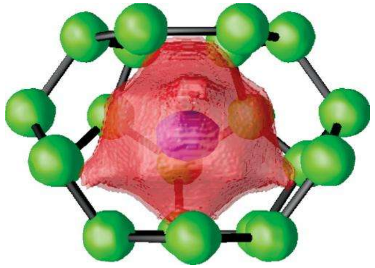
Online Visualization and Simulation Tools for Teaching Nanotechnology

Order of Presentation

- Motivation and Targeted Students
- Visualization & Simulation at the Nanoscale: Need, Methods of Visualizations, & Benefits
- Online Tools for Visualization and Simulations
  - RAIN
  - NanoHub
  - CompuCell3D
- Examples of Visualization in RAIN for user samples and visualization of Viruses
- AFM Overview: Video
- Examples of simulations using nanoHub
- Examples of simulations using CompuCell3D: Simulations of COVID-19
- Conclusion



Visualization and Simulation at the Nanoscale



MOTIVATION

- 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.
- Demand of Global Marketplace: It is predicted that the general need for measurement tools for the emerging field of nanotechnology applications is expected to create a multibillion-dollar market within the next decade.
- Increase knowledge in the field of nanotechnology and STEM education.
- Keeping curricula and labs current with the rapid change of technology pose another challenge for academia.
- Understand the benefits and applications of visualization and simulation at the nanoscale.

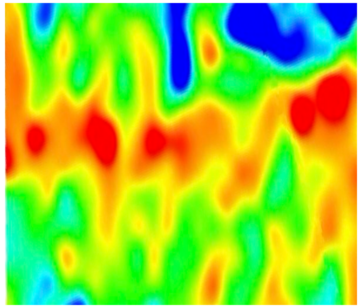
Online Visualization and Simulation Tools for Enhancing Students Learning of Nanotechnology

Targeted Students

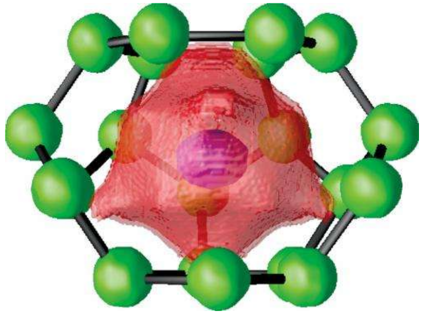
- 4-year Degree programs in engineering , science and engineering technology
- 2-year Associate Degree in engineering, science and engineering technology
- K-12

Suggested Courses

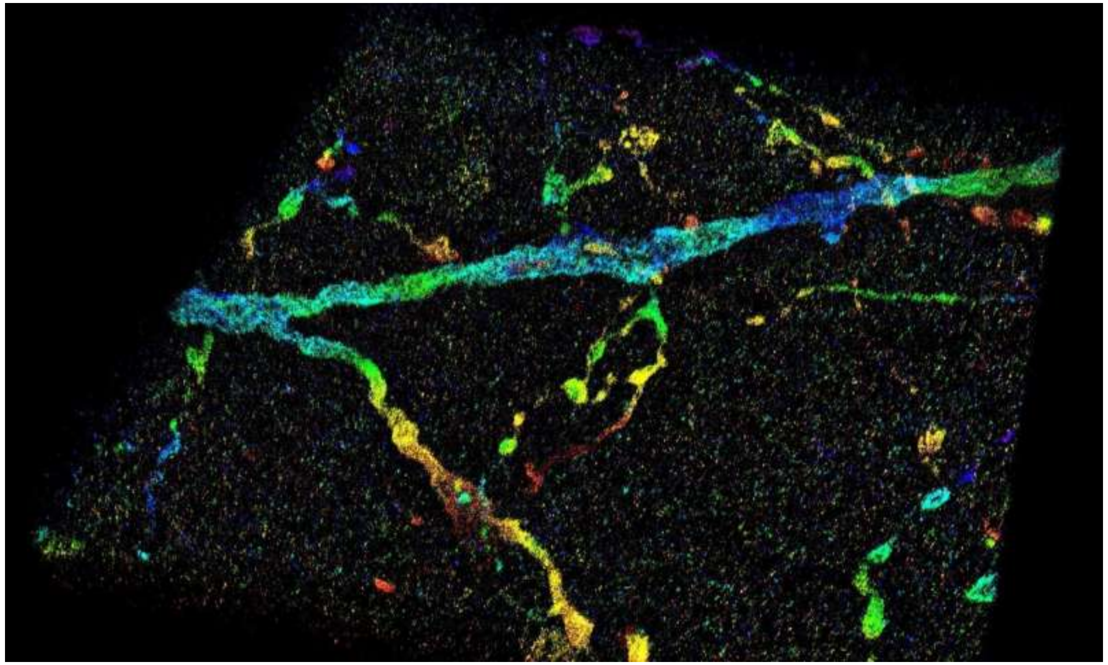
- Introduction to Nanotechnology
- Introduction to Semiconductor Manufacturing
- Material Science
- STEM courses
- Undergraduate/Graduate research and Independent study
- **Micro electromechanical systems (MEMS)**
- **Physics, Chemistry, Engineering, Molecular Biology, Microbiology & and specialized research about Morphologic characterization of Viruses such as Corvid-19**



Need for Visualization at the Nanoscale

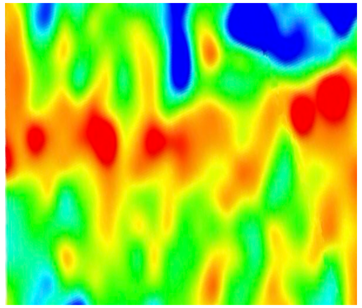


- **Visualization of physical phenomena can confirm hypothesis.**
- **Observation provides opportunities for study without damaging the sample.**
- **Students are motivated by “seeing for themselves”!**

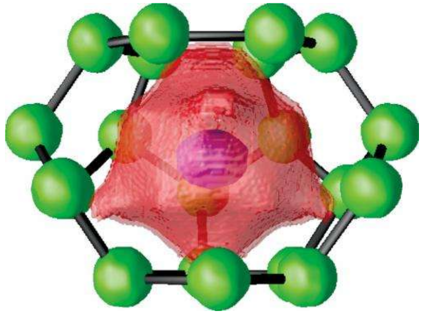


A 3-D super-resolution reconstruction of dendrites in primary visual cortex.

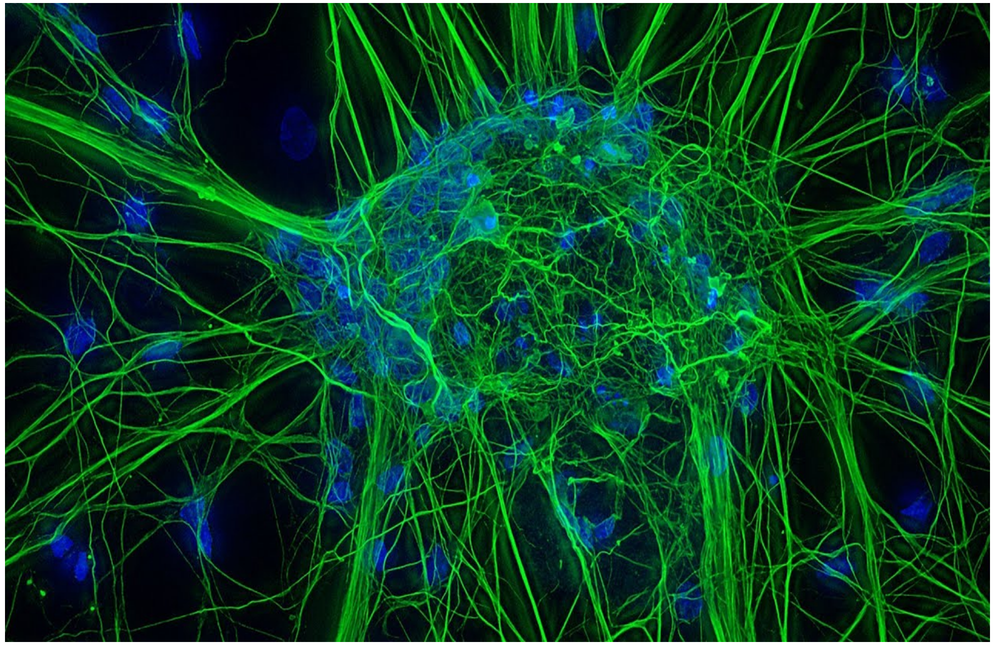
https://phys.org/news/2020-05-imaging-technology-visualization-nanoscale-cells.html



Need for Visualization at the Nanoscale

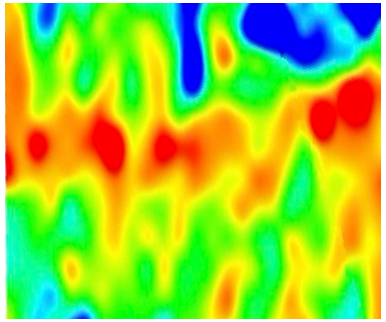


- Morphologic characterization of Viruses such as Corvid-19.
- Development of new products requires visualization coupled with interfacial interactions, and measurement at the nanoscale.
- Objects under study may be too small for our hands to handle or manipulate.



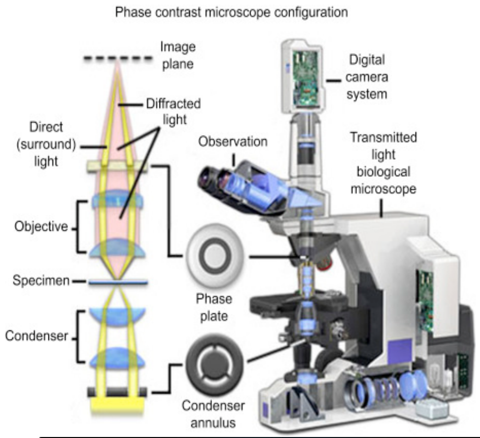
THUNDER Imager 3D Live Cell & 3D Cell Culture - Decode 3D Biology in Real Time*

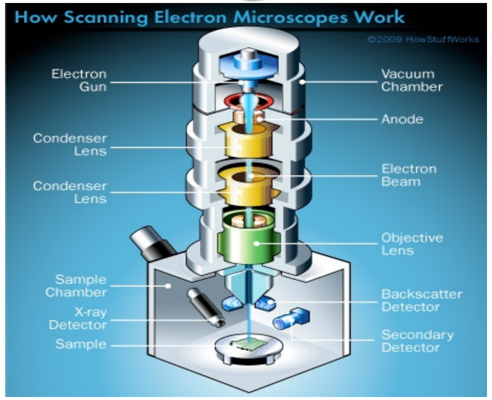
https://i.ytimg.com/vi/Bq2f9FDIZJ4/maxresdefault.jpg

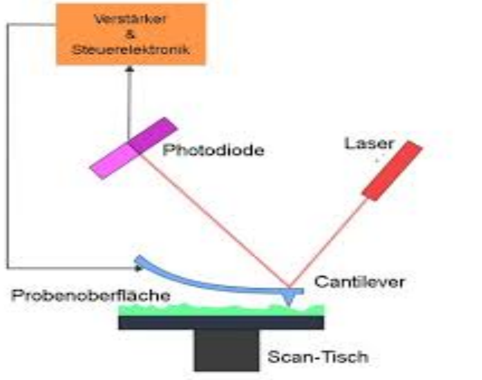


Methods of Nanoscale Visualization

- **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.







Visualization and Simulation at the Nanoscale

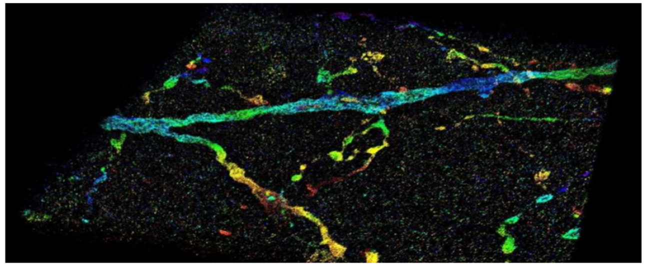
Visualization of processes can be achieved by using laboratory instruments, online simulation and remote access instruments.

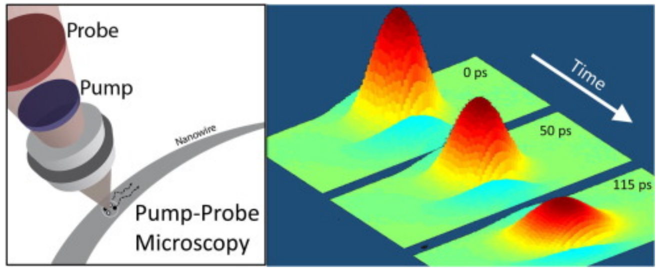
Online Tool/Methods of Visualizations and Simulation at the Nanoscale:

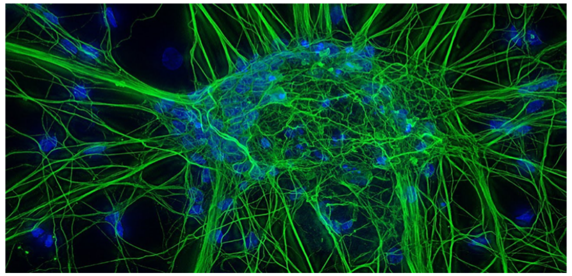
- Remote Accessible Instruments for Nanotechnology (RAIN)
- NoanoHUB: www.nanohub.org
- CompuCell 3D https://compucell3d.org

Benefits

- **Saving on buying an expensive equipment**
- **Helps to train students before buying the equipment**
- **Introduce students to the field of nanotechnology**







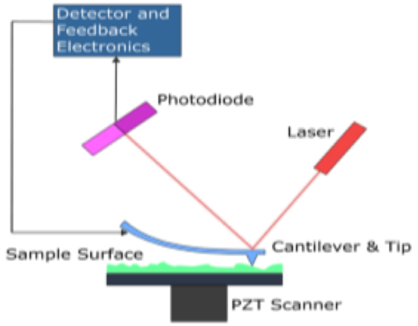
Learning through Visualization at the Nanoscale

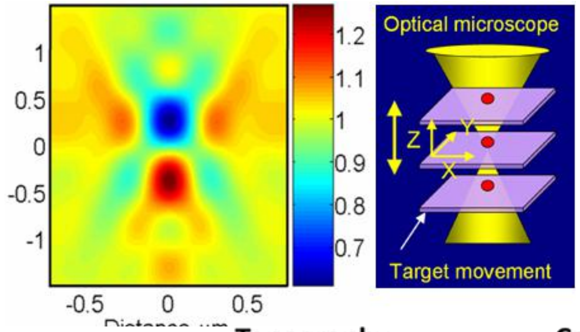
Types of Tools at RAIN

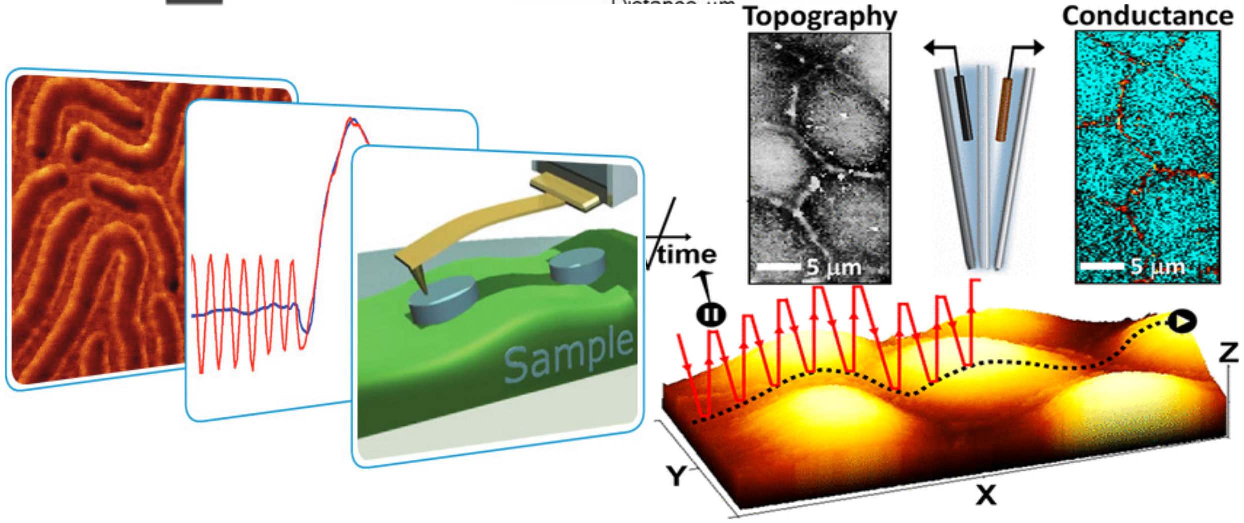
RAIN allows students to access and control microscopes and analytical tools, to look at nanosized materials from the ease of classrooms, or home computers, across the country.

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







Remote Accessibility of Nanotechnology Instruments

Atomic Force Microscope (AFM)

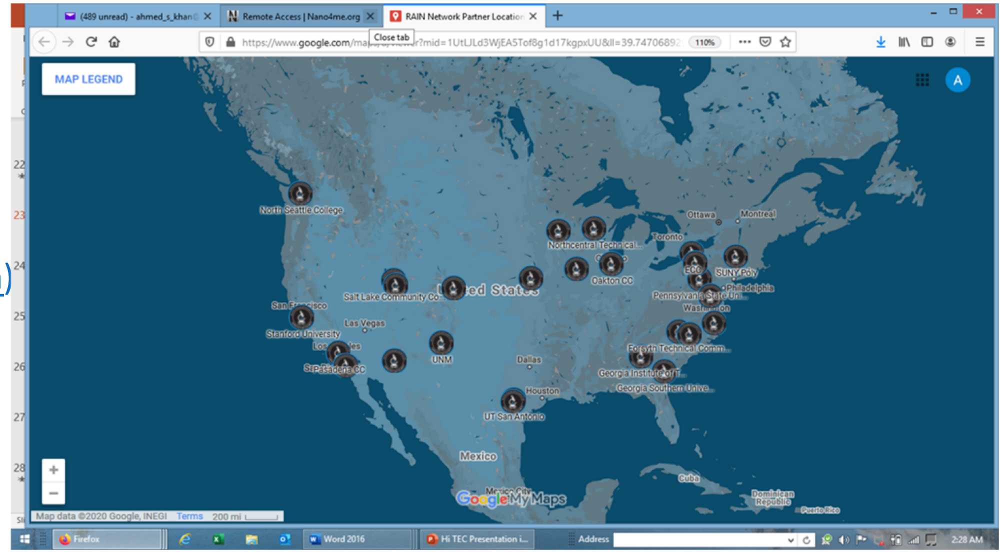
- Forsyth Tech Community College - (Nanosurf Flex Scan head AFM)
- Northcentral Technical College - (Nanosurf easyScan 2)
- North Seattle College - (Nanosurf easyScan 2)
- Oakton Community College - (Nanosurf easyScan 2 FlexAFM)
- Pennsylvania State University - (Bruker Innova)
- Salt Lake Community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

Scanning Electron Microscope (SEM)

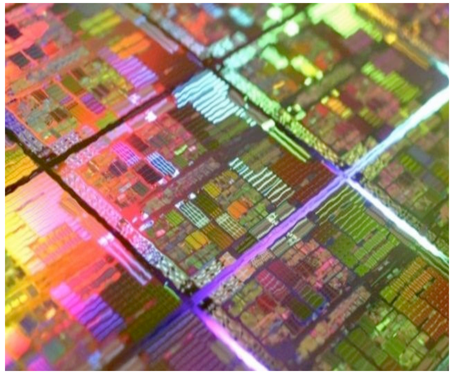
- NCI-SW at Arizona State University - (Phenom Pro)
- CABOCES - (Phenom ProX & JEOL-JSM-6010PLUS/LA)
- Erie Community College - (JEOL JSM-6010LA)
- Northcentral Technical College - (Hitachi TM 3030)
- Oakton Community College - (Hitachi TM 3000)
- North Seattle College - (Aspex EXplorer)
- Pasadena City 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

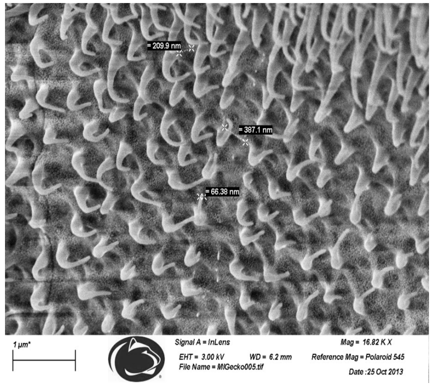
- Pennsylvania State University - (Leitz Ergolux)



Examples of Nanoscale images captured with the tools available for online the users at RAIN



Microchip



Gecko

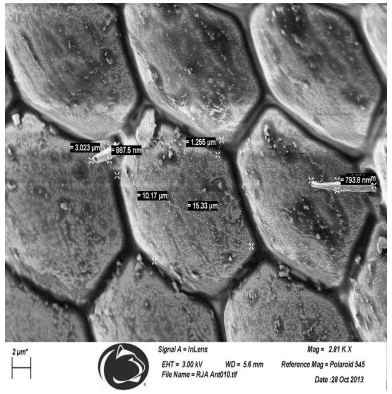
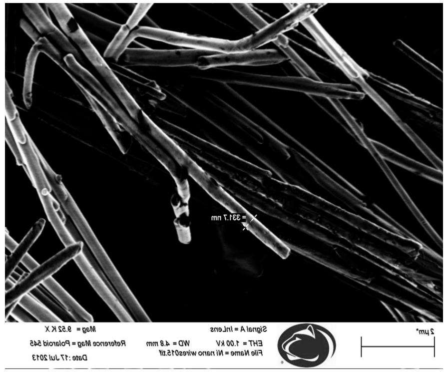
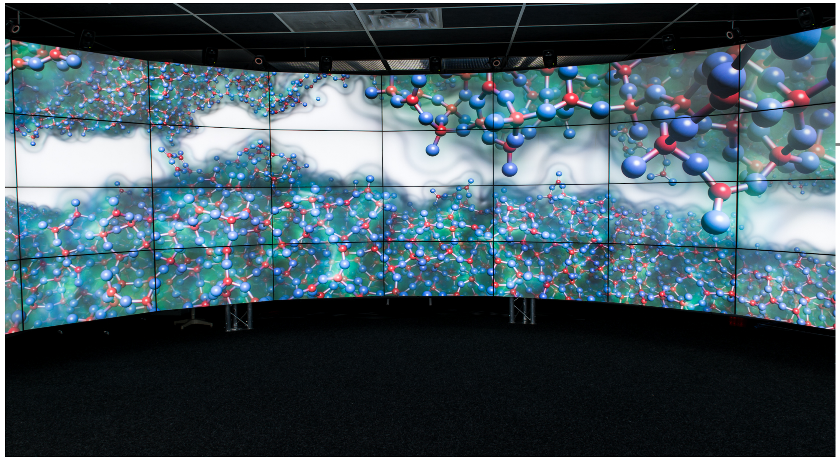


Image of Ant



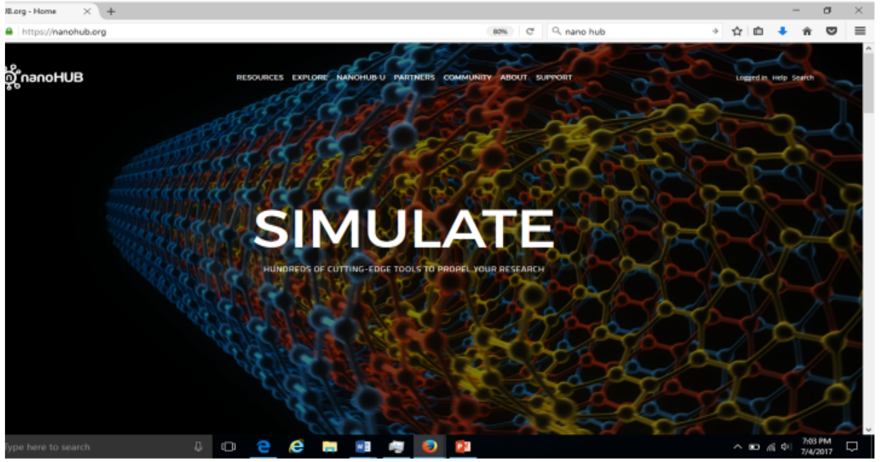
Ni Nano wires

Learning through Simulation at the Nanoscale



Crystal Viewer Tool

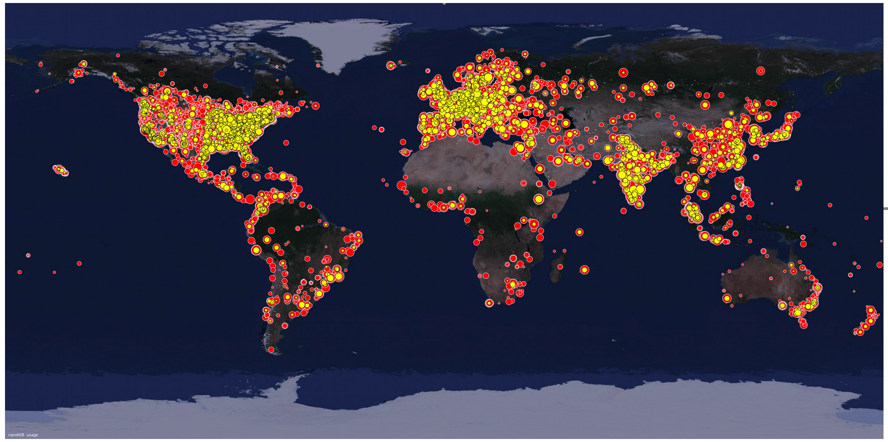
Nanohub.org



Simulation offers several additional advantages:

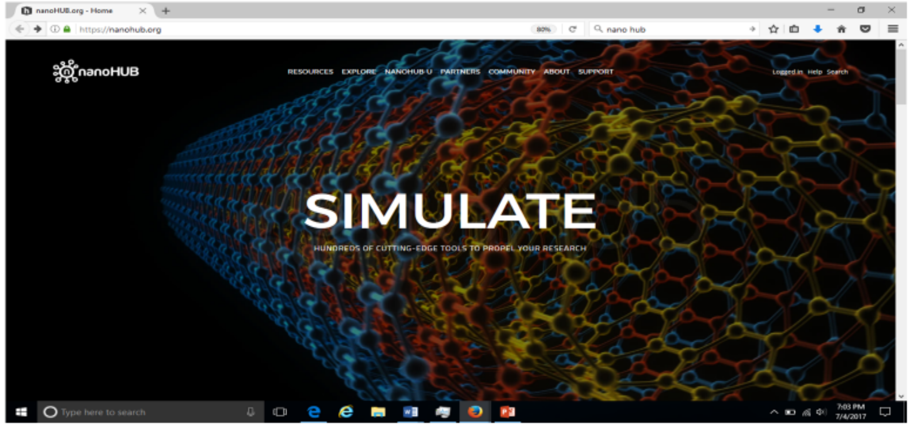
1. Allowing the user to modify system parameters and observe the outcomes without any harmful side effects
2. Eliminating component or equipment faults that affect outcomes
3. Supporting users progress at their own pace in discovery and understanding of concepts and issues
4. Enhancing the presentation of "dry" concepts by integrating theory and practice

Simulation Tools at the Nanoscale
NanoHub.org



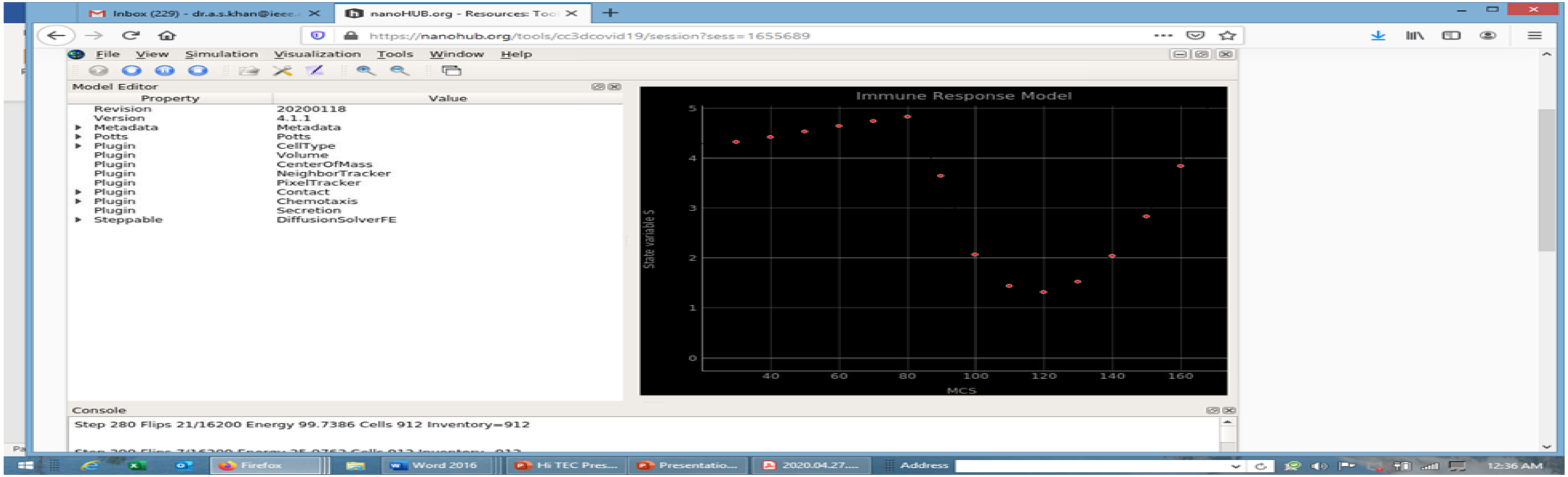
- Computing Cloud located at Purdue University
- 500+ simulation tools
- 1.4 million users Worldwide
- 5500 resources
- The COVID-19 simulation can also be run online without requiring any installations or downloads on the nanoHUB

Crystal Viewer Tool
Nanohub.org

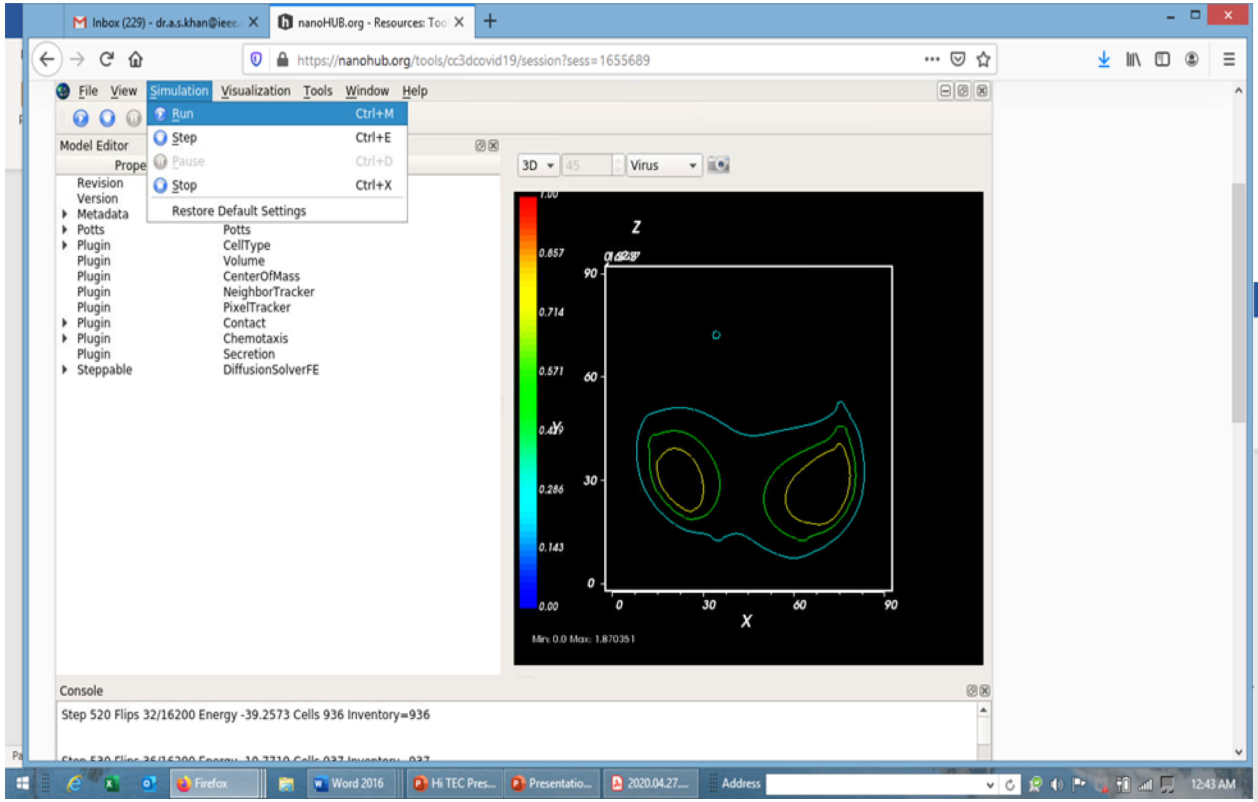


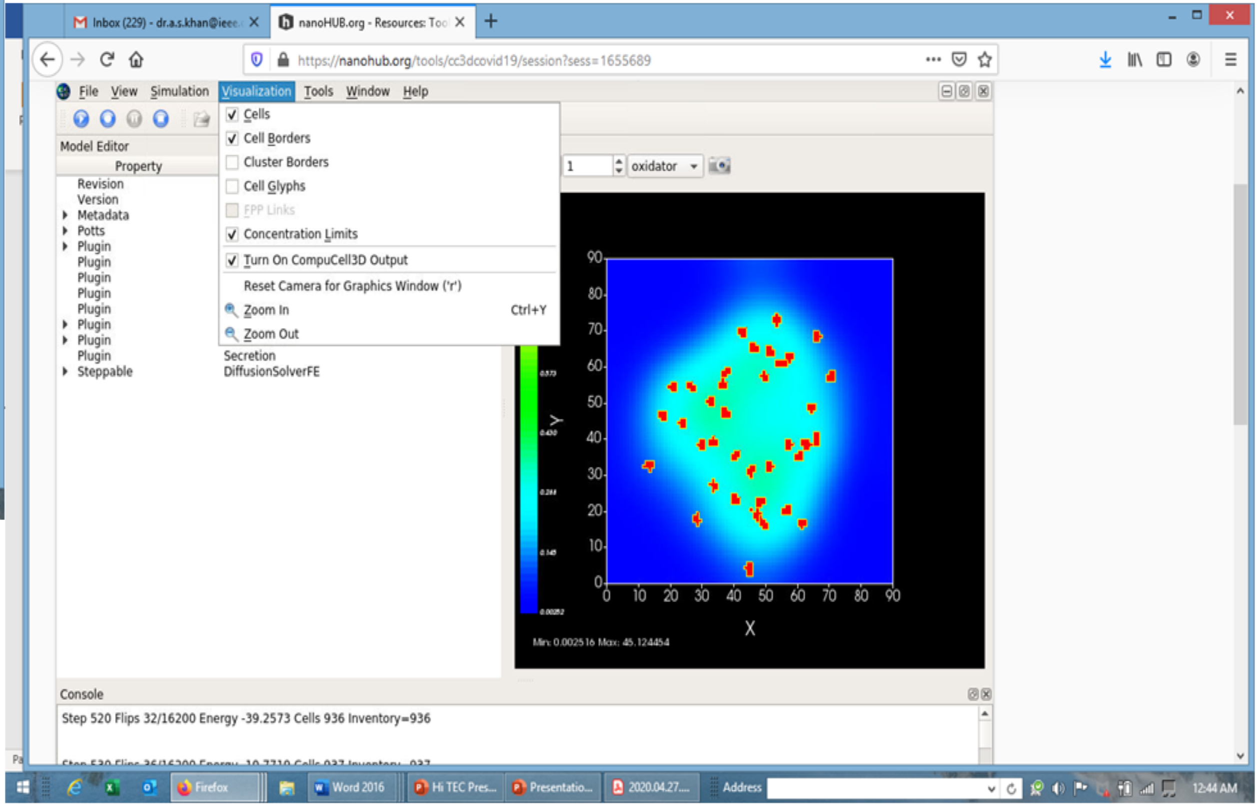
CompuCell3D

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.



CompuCell3D





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

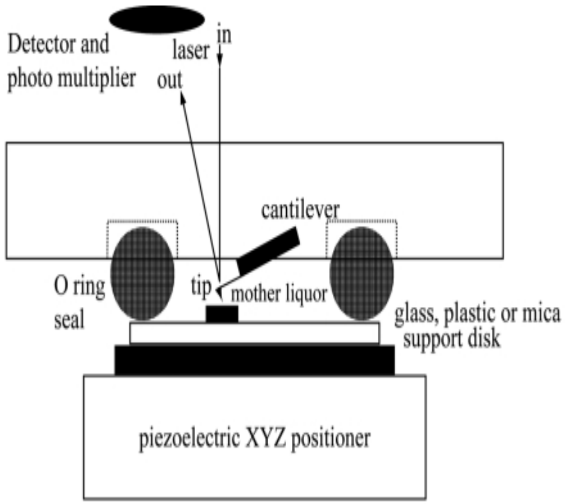
Part-II: Video

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

CompuCell3D can be downloaded from https://compucell3d.org/SrcBin

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)*



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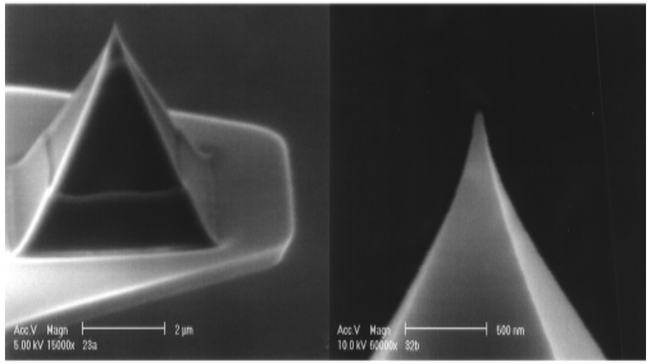

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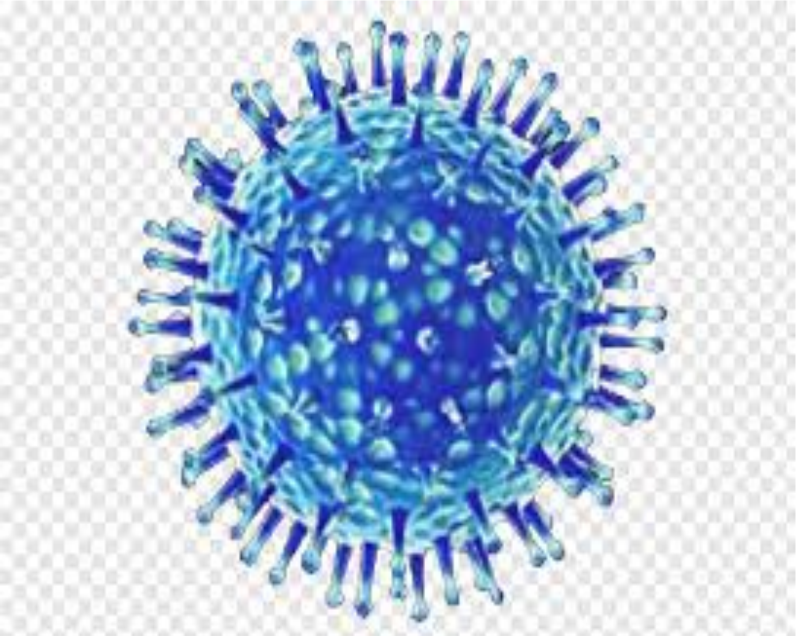
Detection of Viruses using Nanoscale Visualization

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**

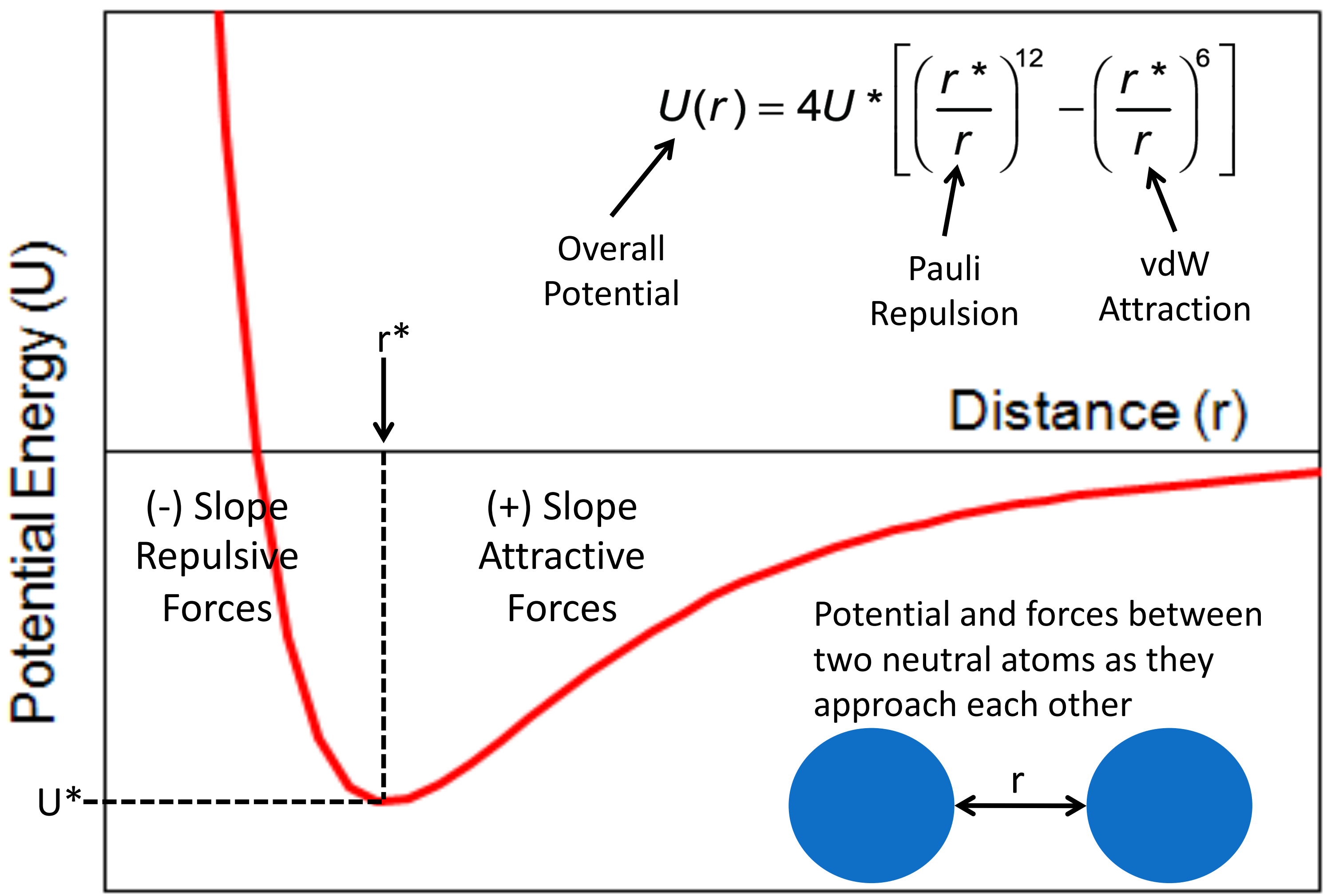
These techniques require expensive equipment, difficult to install and cannot be used for live biological samples as compared to Atomic Force Microscopes which is inexpensive, easy to install, smaller in size with additional features.

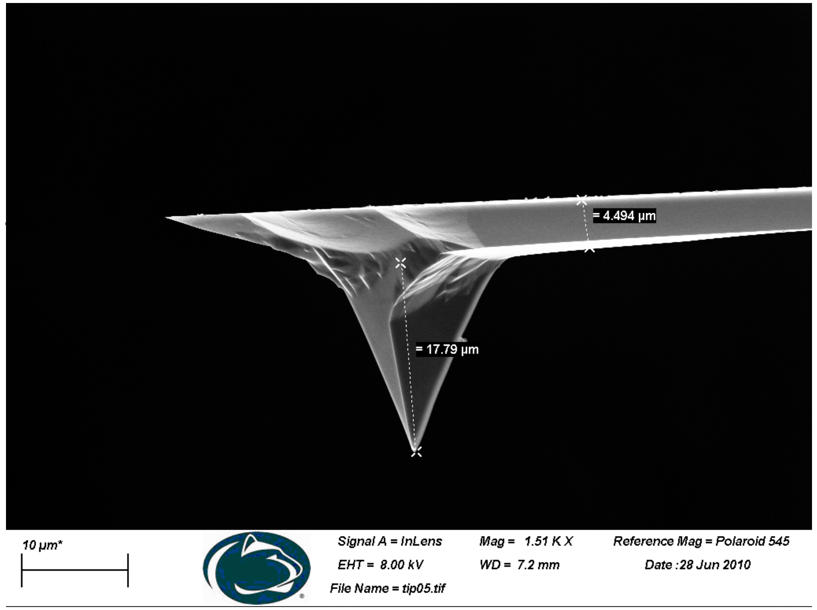


Avian influenza Virus Common cold Infection, dentate bacterial virus PNG

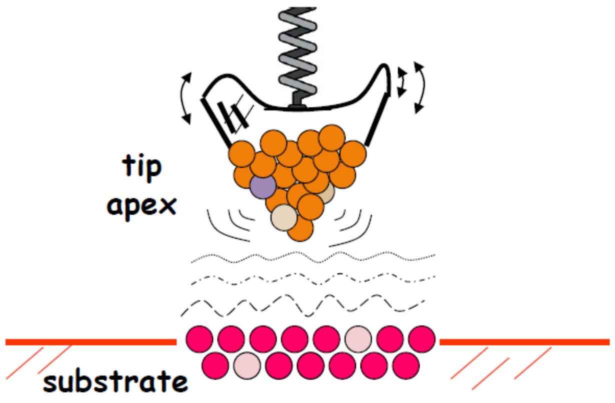
AFM Overview

Intermolecular Forces



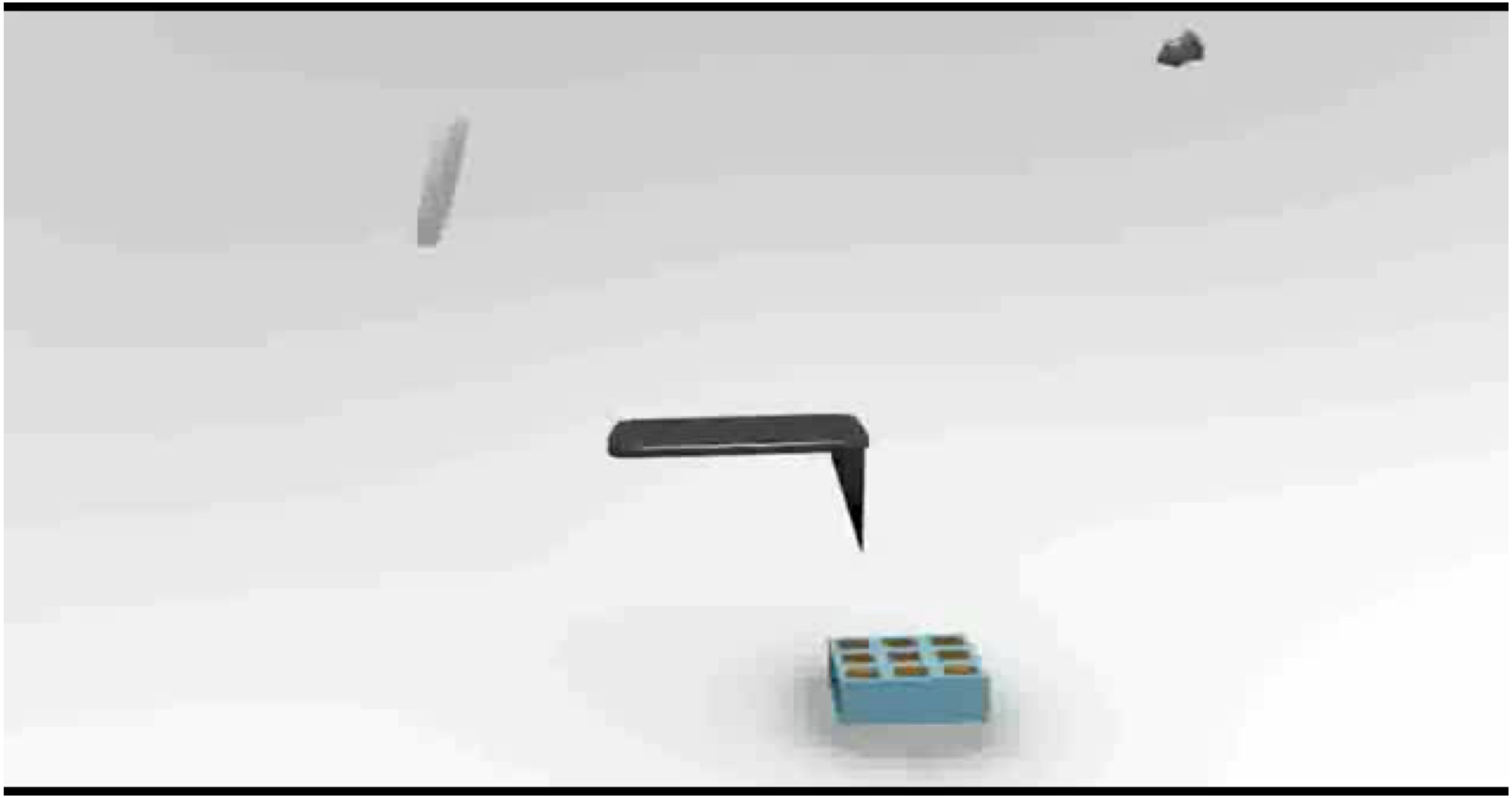


Atom-Atom?



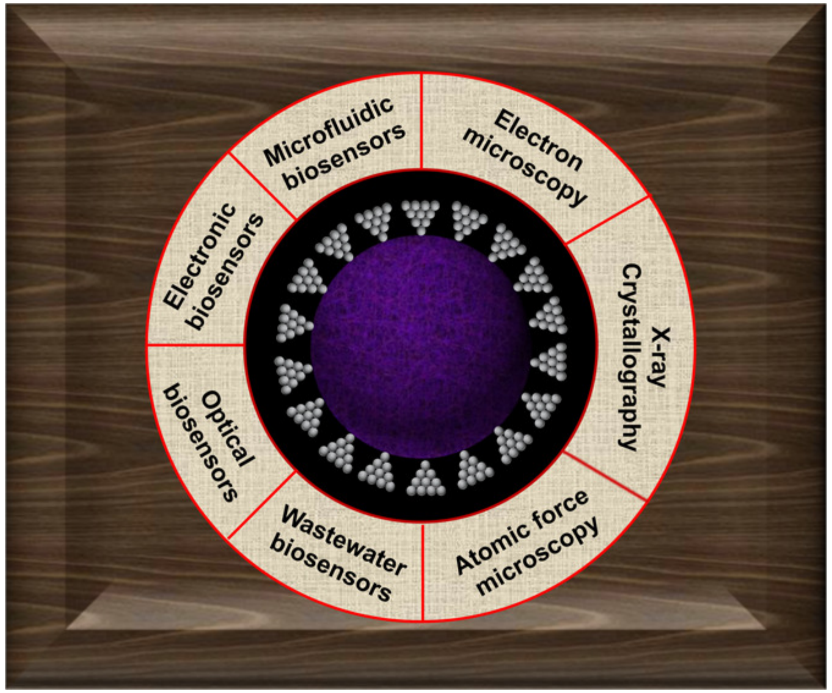
AFM Overview: Video

Please place the cursor in the center then click on play button.



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.



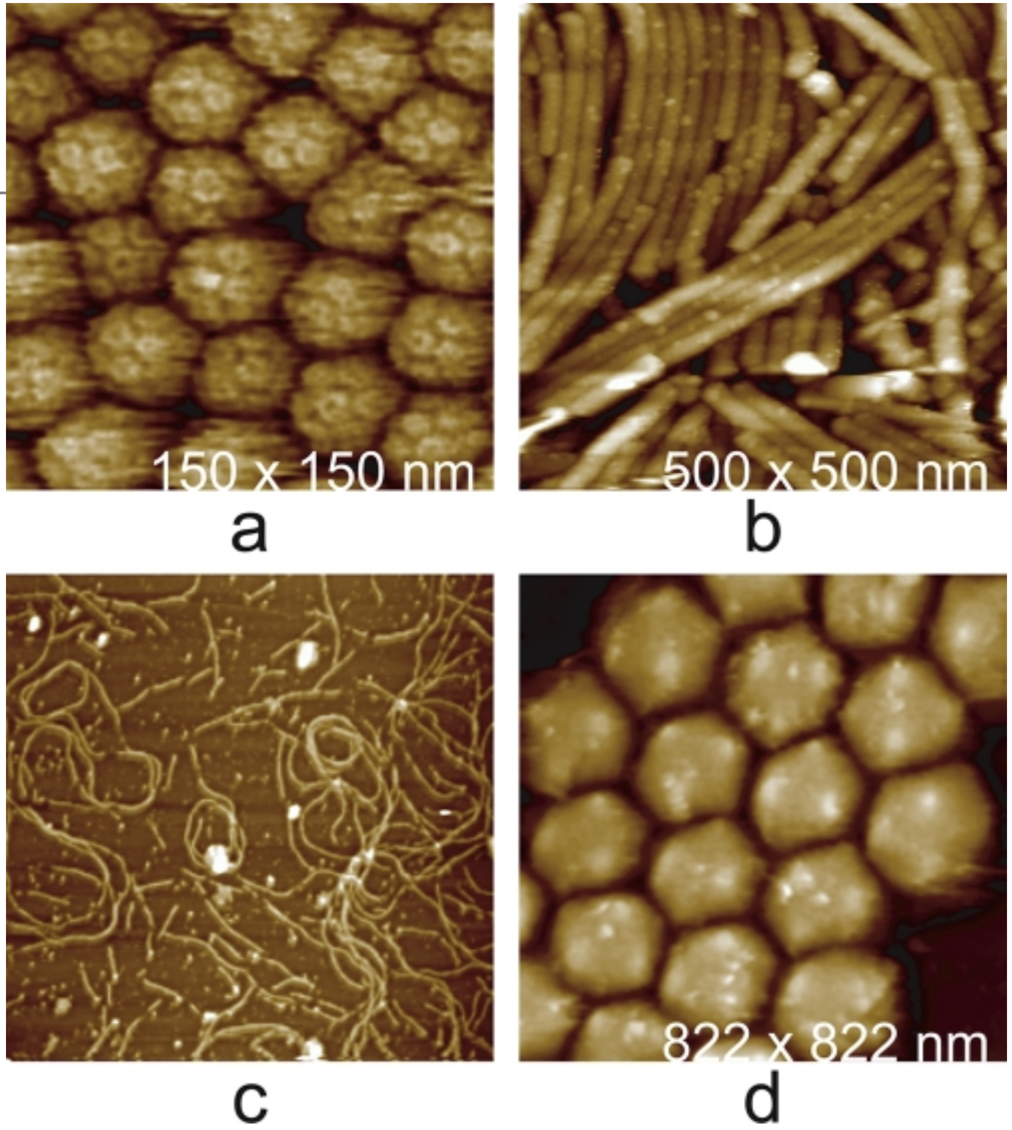
Opportunities and Challenges for Biosensors and Nanoscale Analytical Tools for Pandemics: COVID-19*

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

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

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.

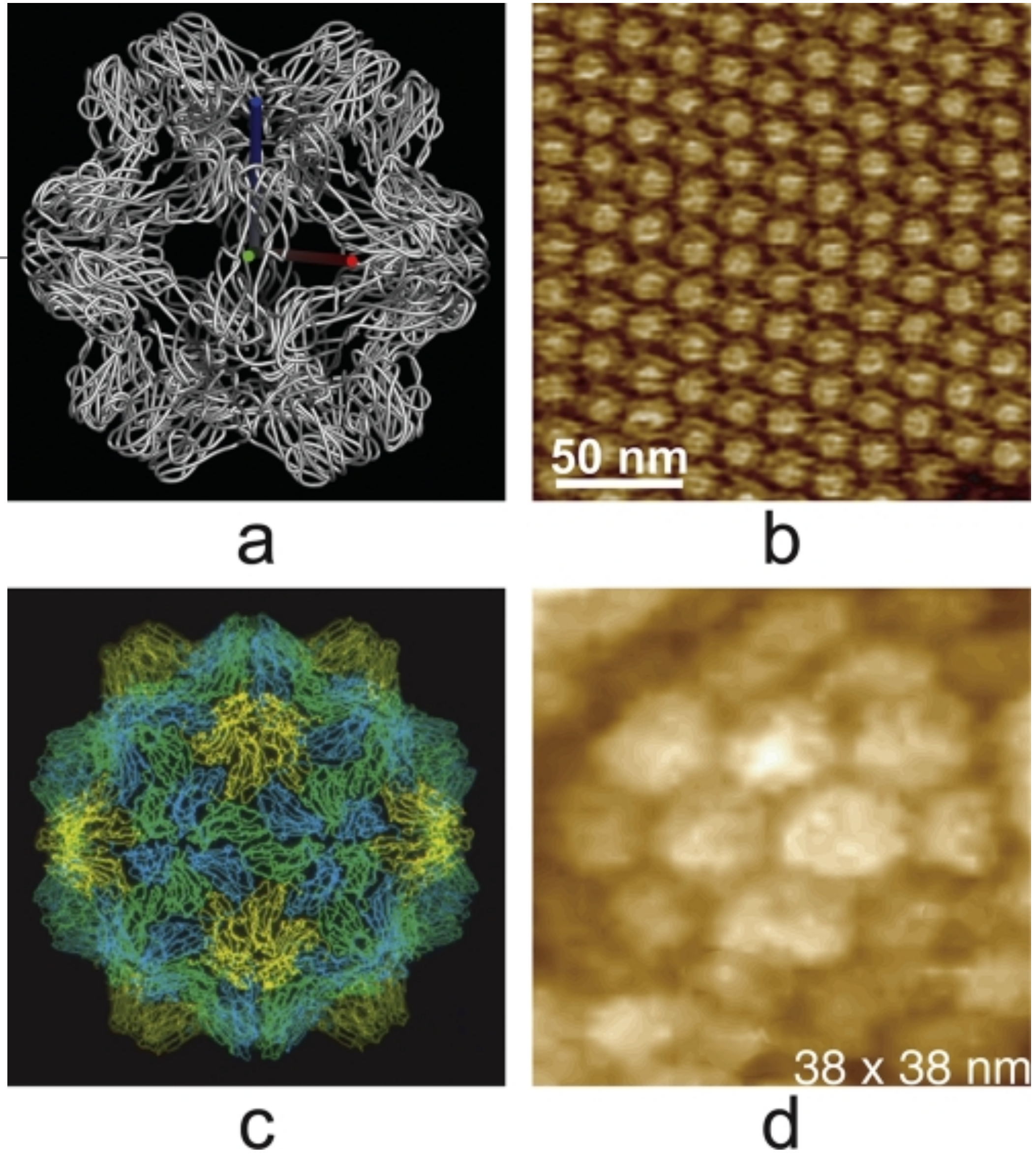


***Atomic Force Microscopy in Imaging of Viruses and Virus-Infected Cells**

Yurii G. Kuznetsov and Alexander McPherson*

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

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



(a) Polypeptide backbone structure, determined by X-ray crystallography, of the T = 1 particle that forms when the T = 3 virion of brome mosaic virus is treated with high salt and neutral pH. It is seen looking along a 2-fold axis. (b) Surface of a crystal of the BMV T = 1 particles. (c) Polypeptide backbone structure of the T = 3 icosahedral turnip yellow mosaic virus, also determined by X-ray diffraction analysis. (d) A single virion of TYMV, imaged by AFM, which was incorporated into the surface of a crystal of the virus. The pentameric and hexameric capsomeres are evident in the AFM image.

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

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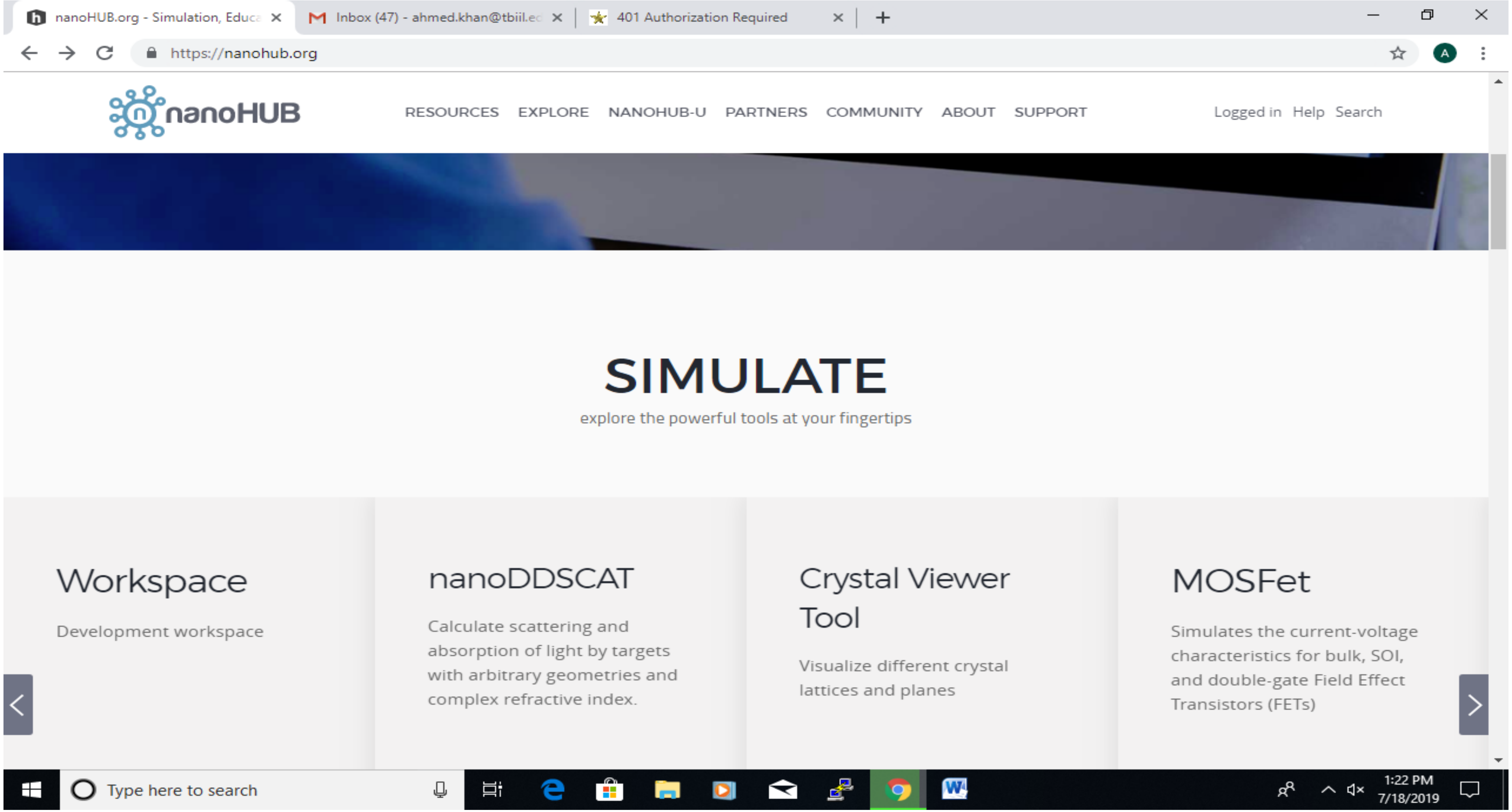
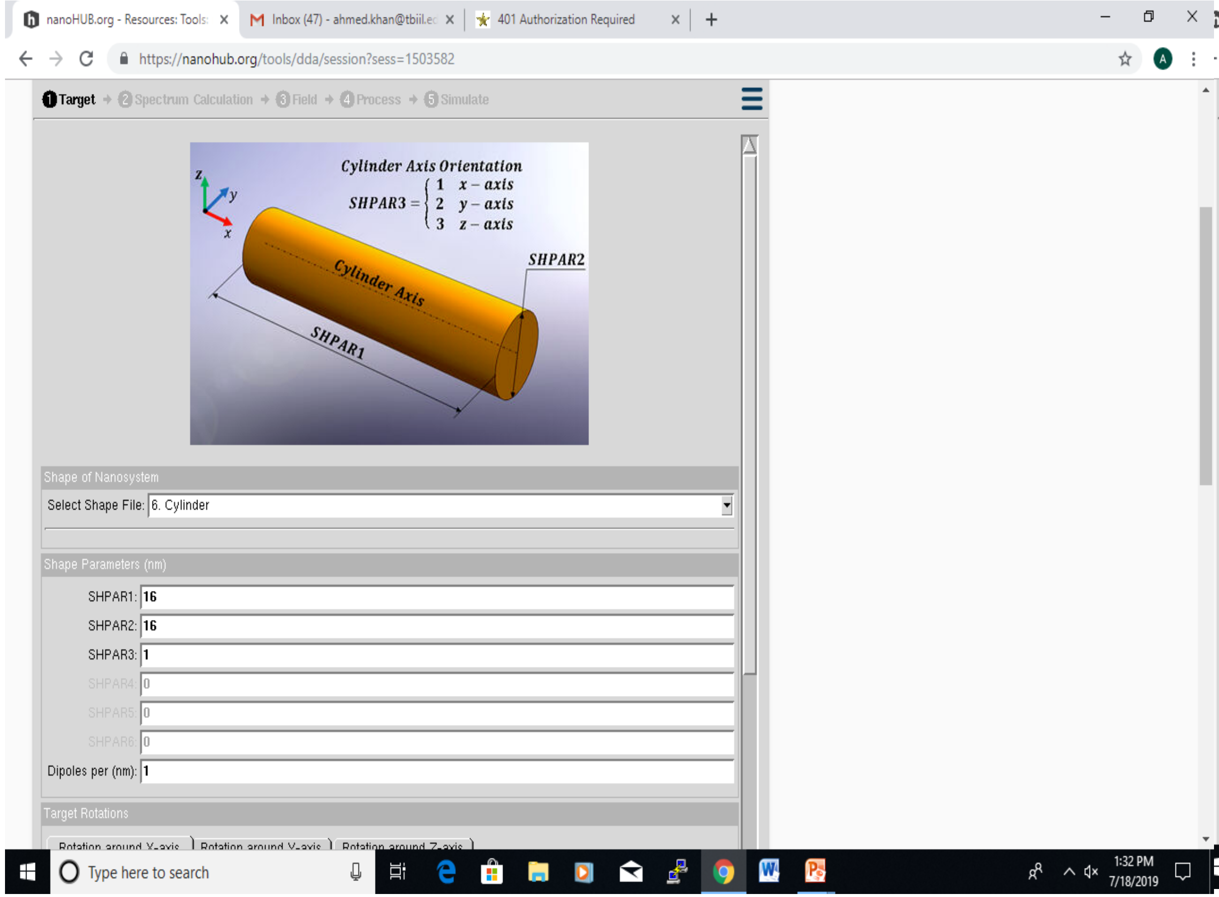
NanoHub Simulation Tools



Examples of NanoDDSCAT using nanoHub

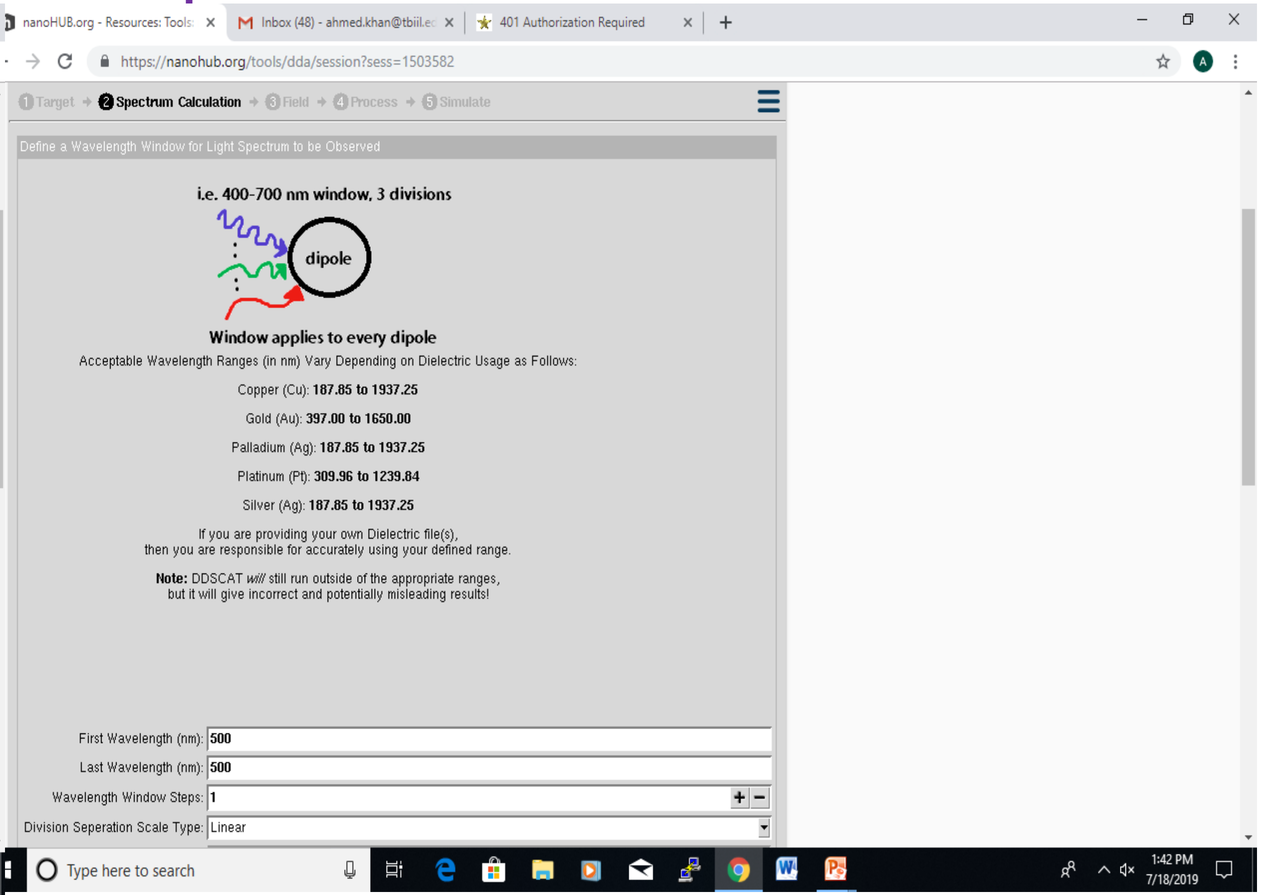
Calculate scattering and absorption of light with arbitrary geometry and complex Refractive Index

1. Target



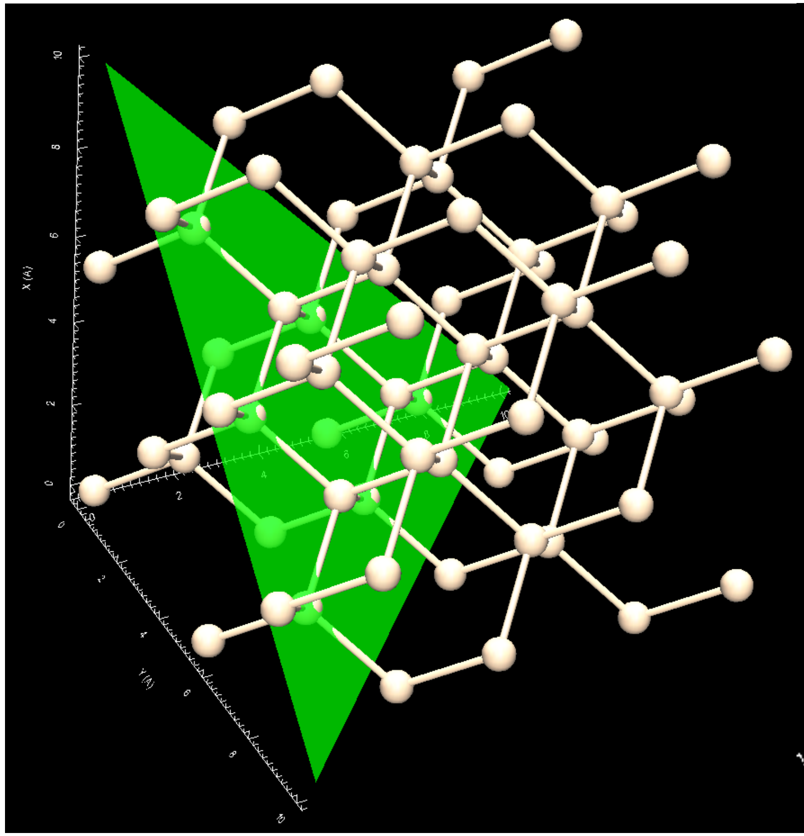
Calculate scattering and absorption of light with arbitrary geometry and complex Refractive Index

2. Spectrum Calculation

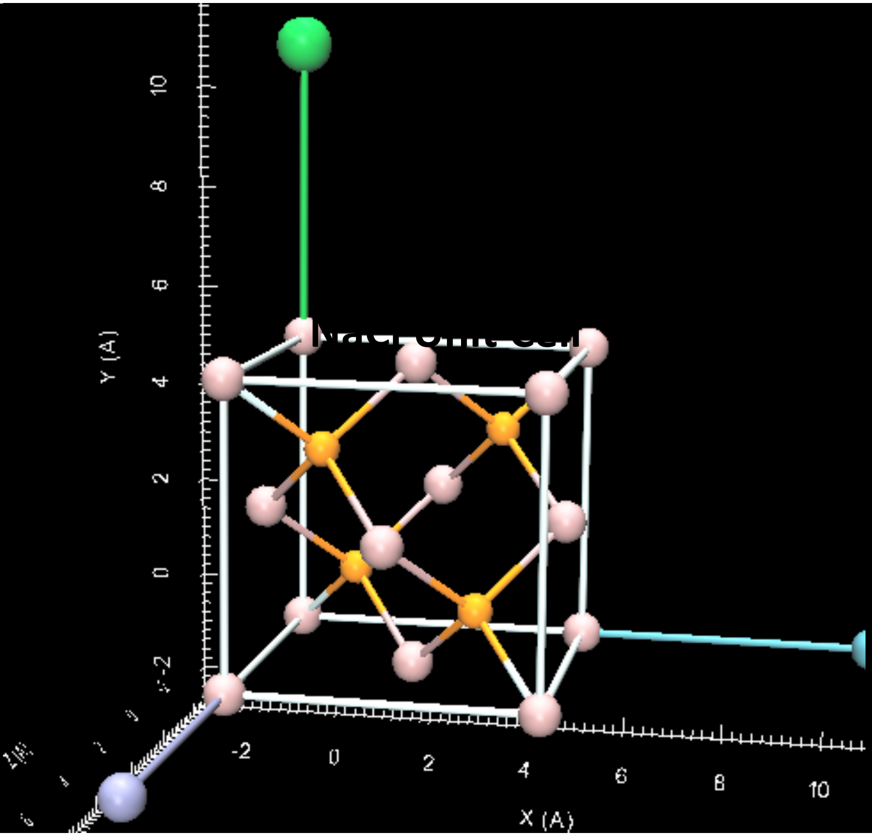


Examples of Crystal Viewer simulation tool using nanoHub for:

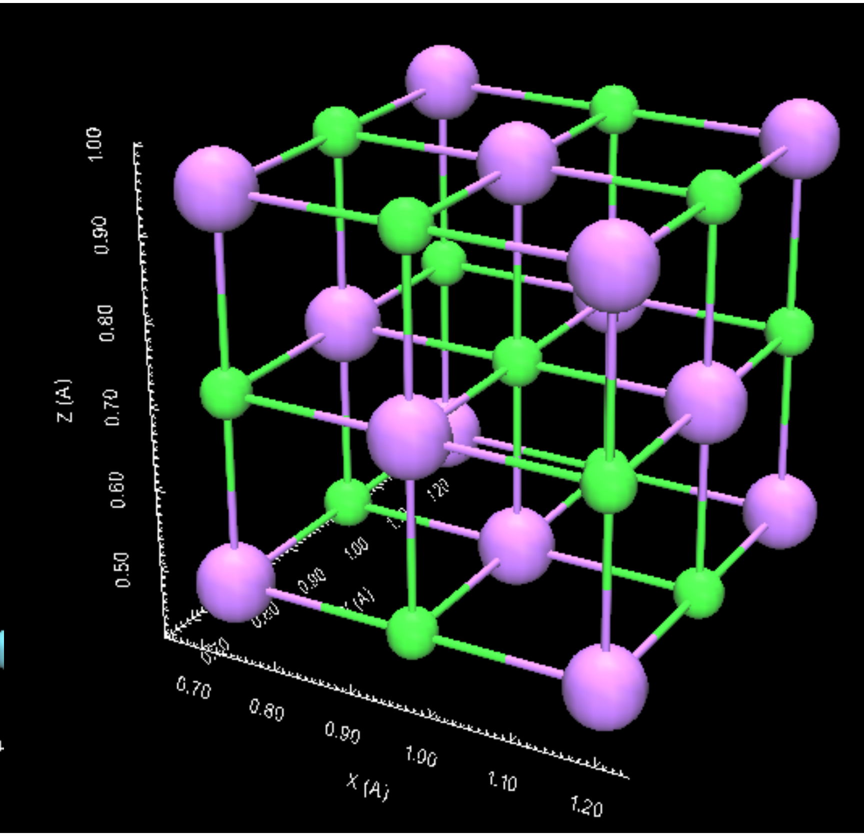
(a) viewing all materials which have periodical structure
(b) building crystal structure even not exists in nature



Silicon With Miller Plane

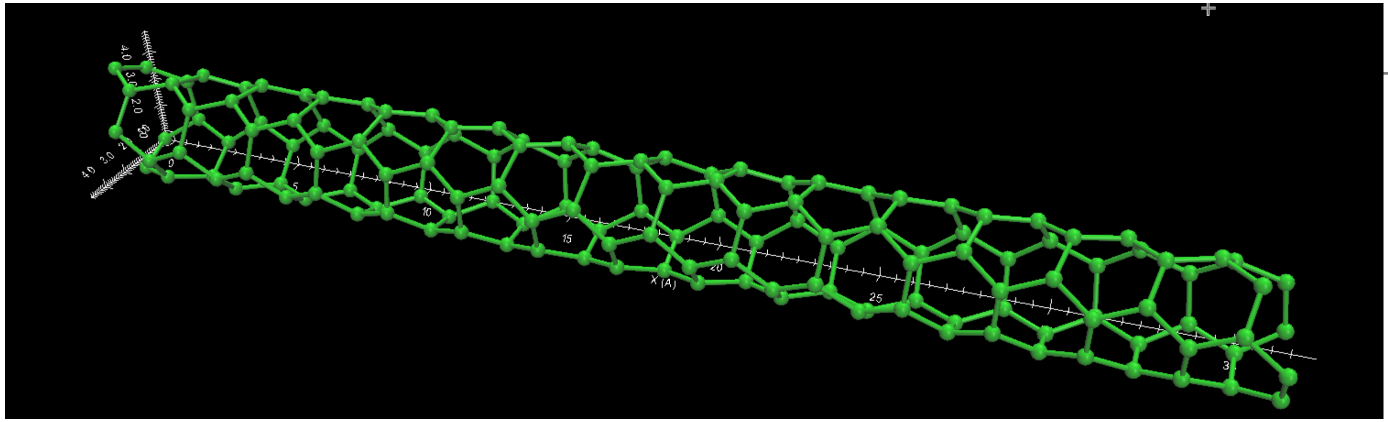


GaP Unit Cell

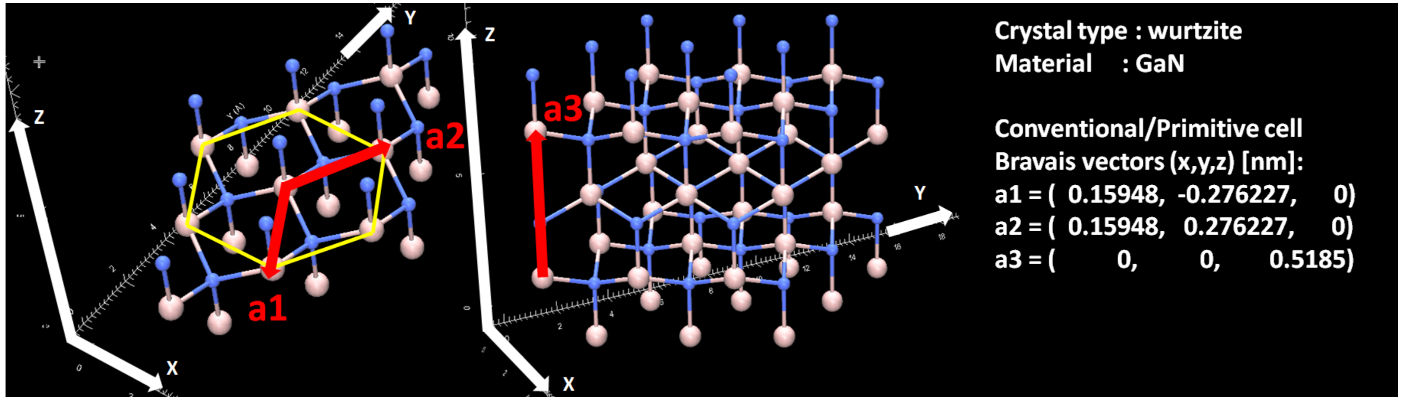


NaCl Unit Cell

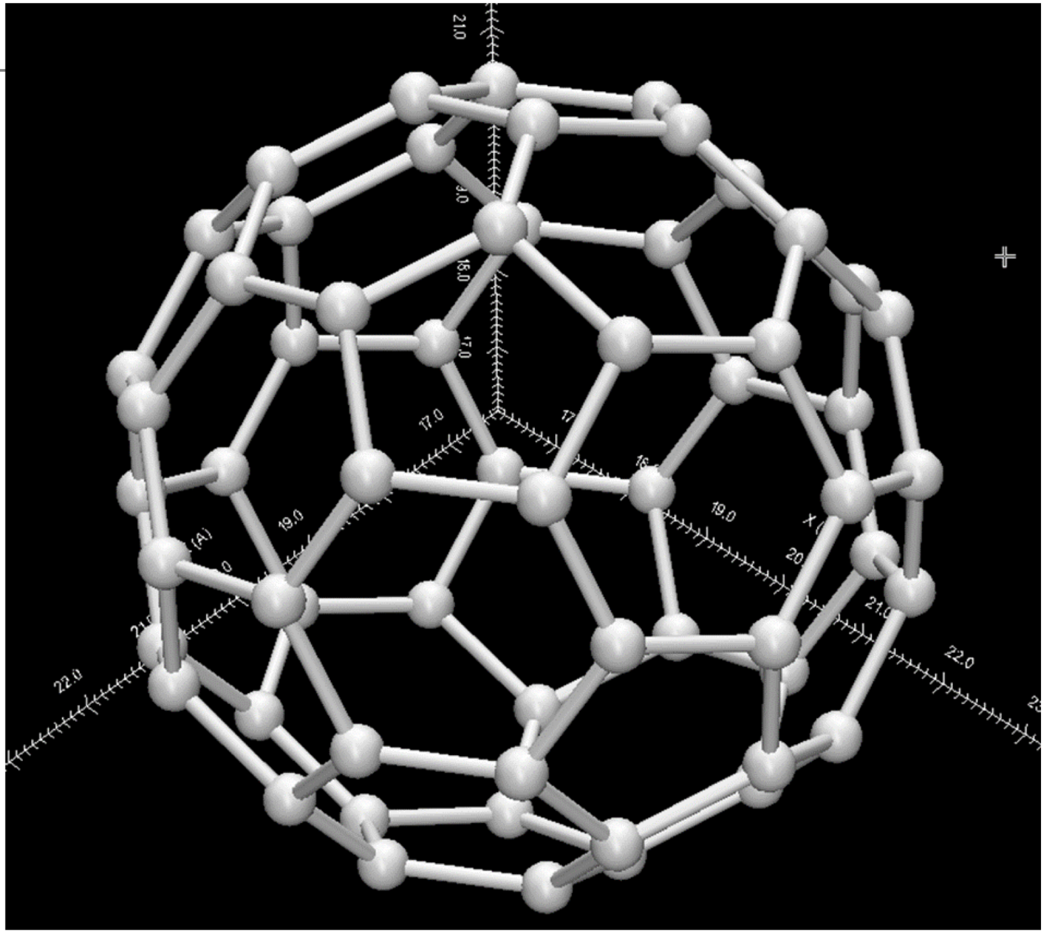
Examples of Nano Structure Visualization with nanoHub's Crystal Viewer



Carbon nano tube



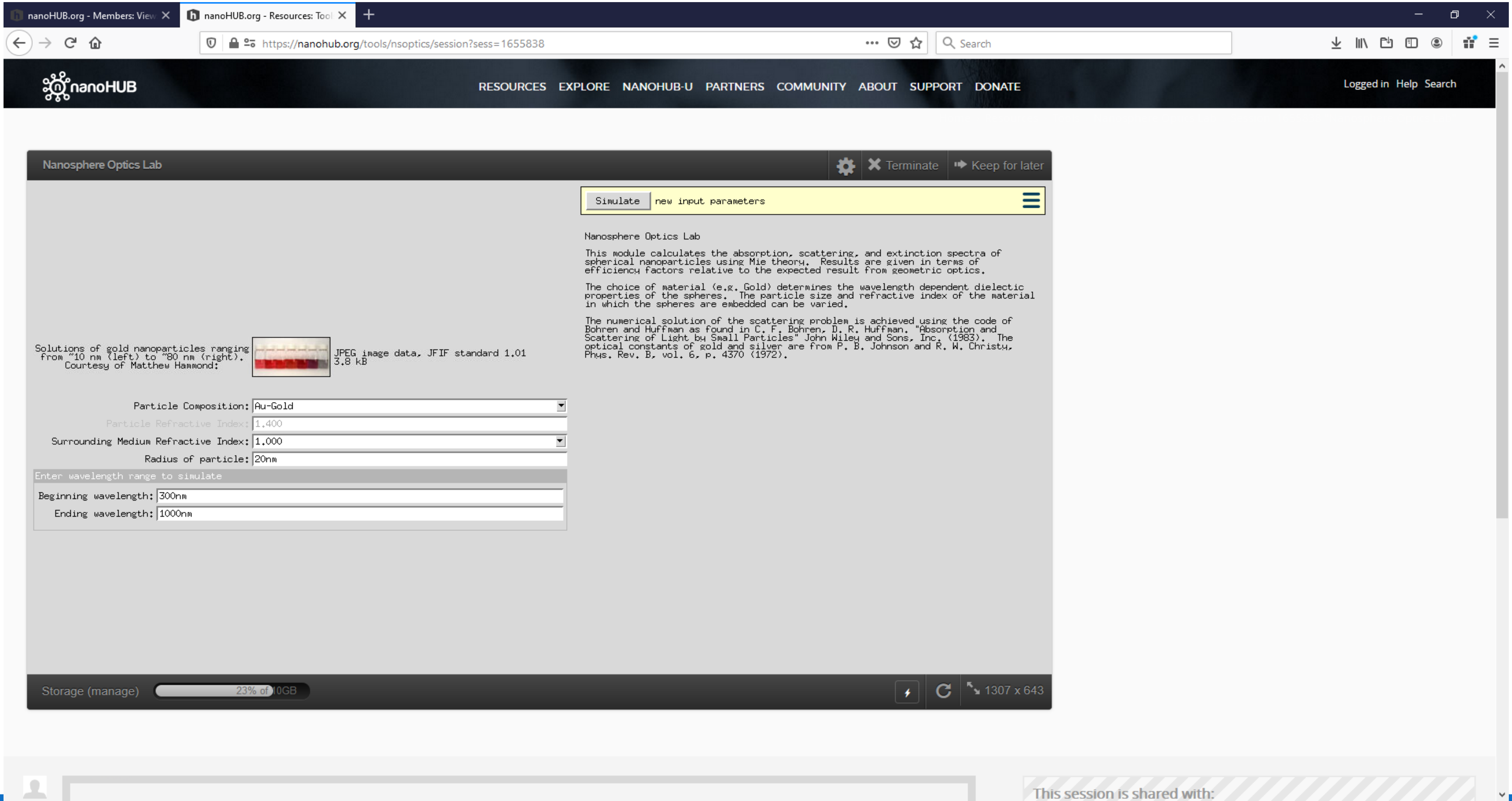
GaN Bravais Vectors



Buckey Ball

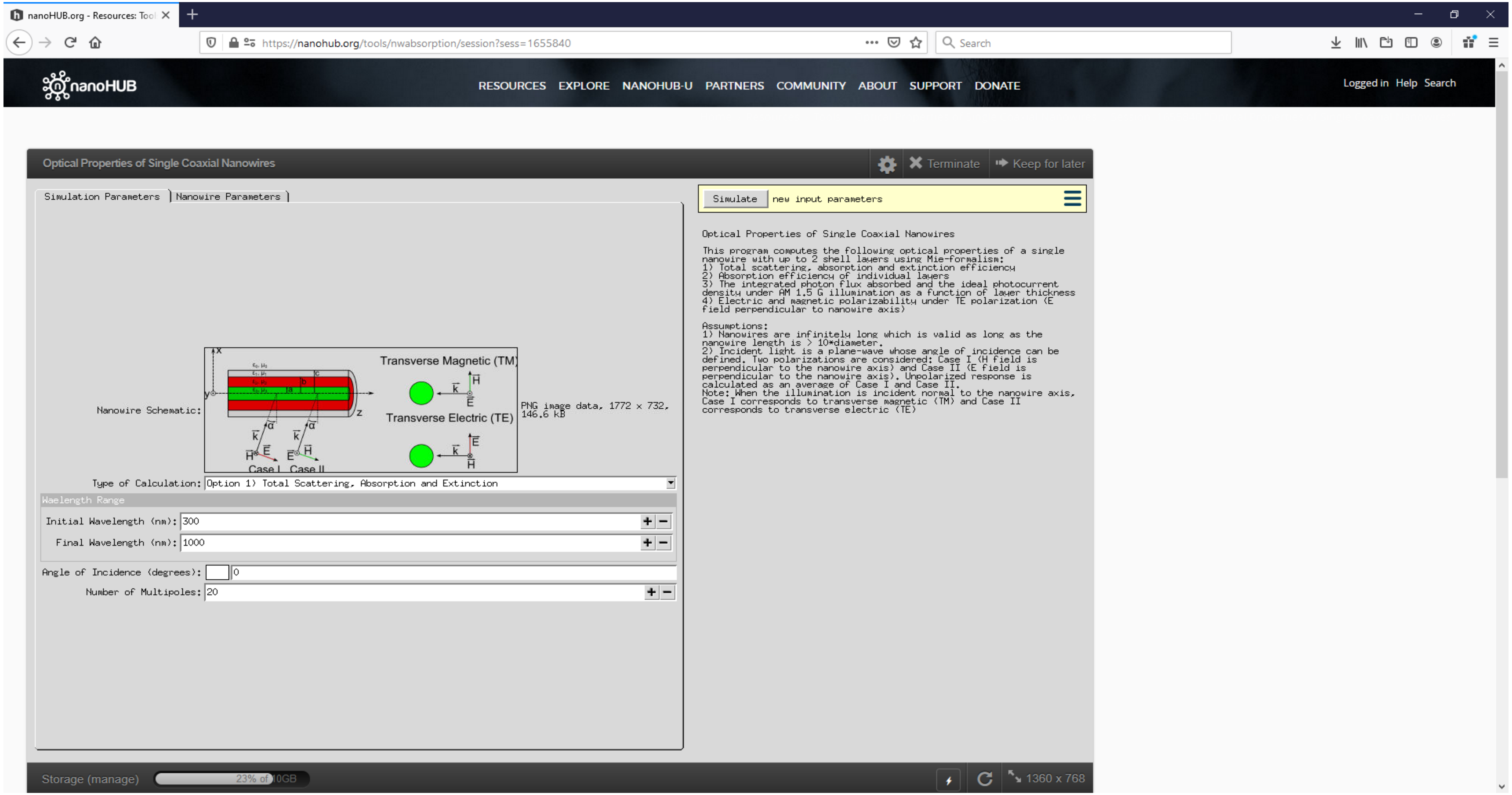
Nanosphere Optics Lab over NanoHub

Calculate absorption from metallic nanoparticles



Nanosphere Optics Lab over NanoHub

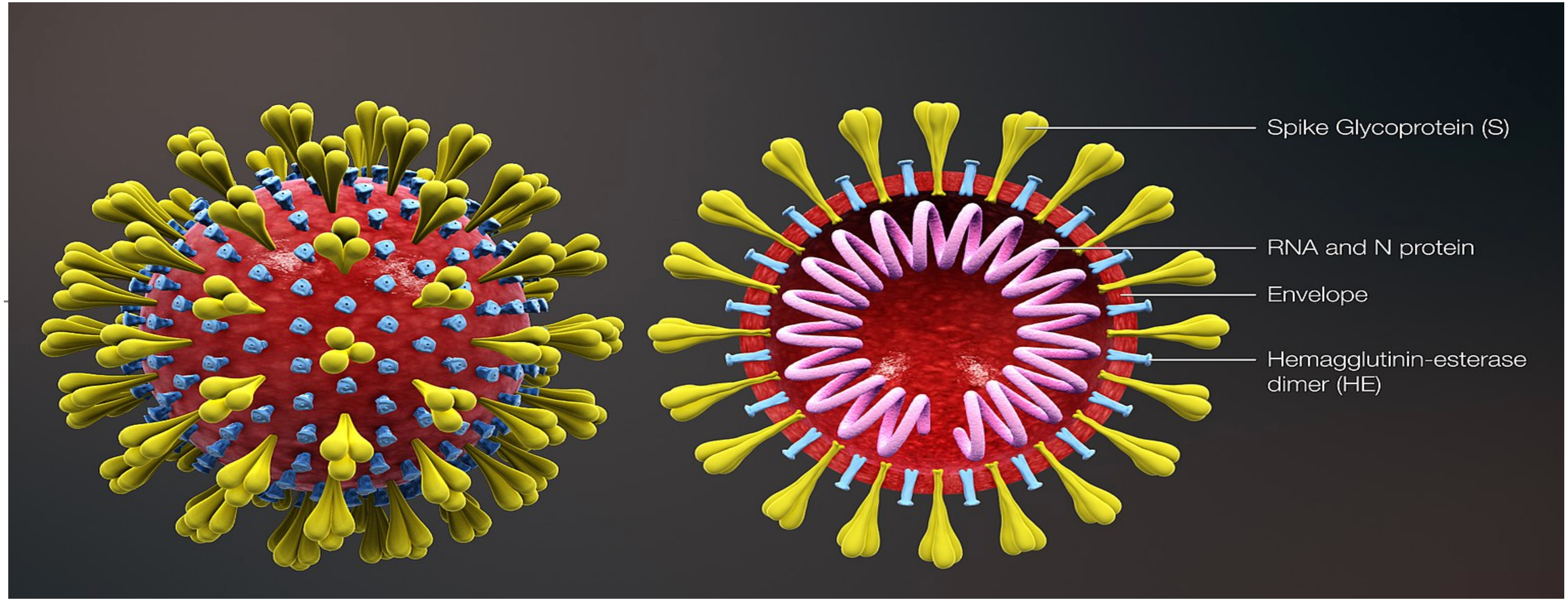
Calculate absorption and scattering from single nanowires with or without shells



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



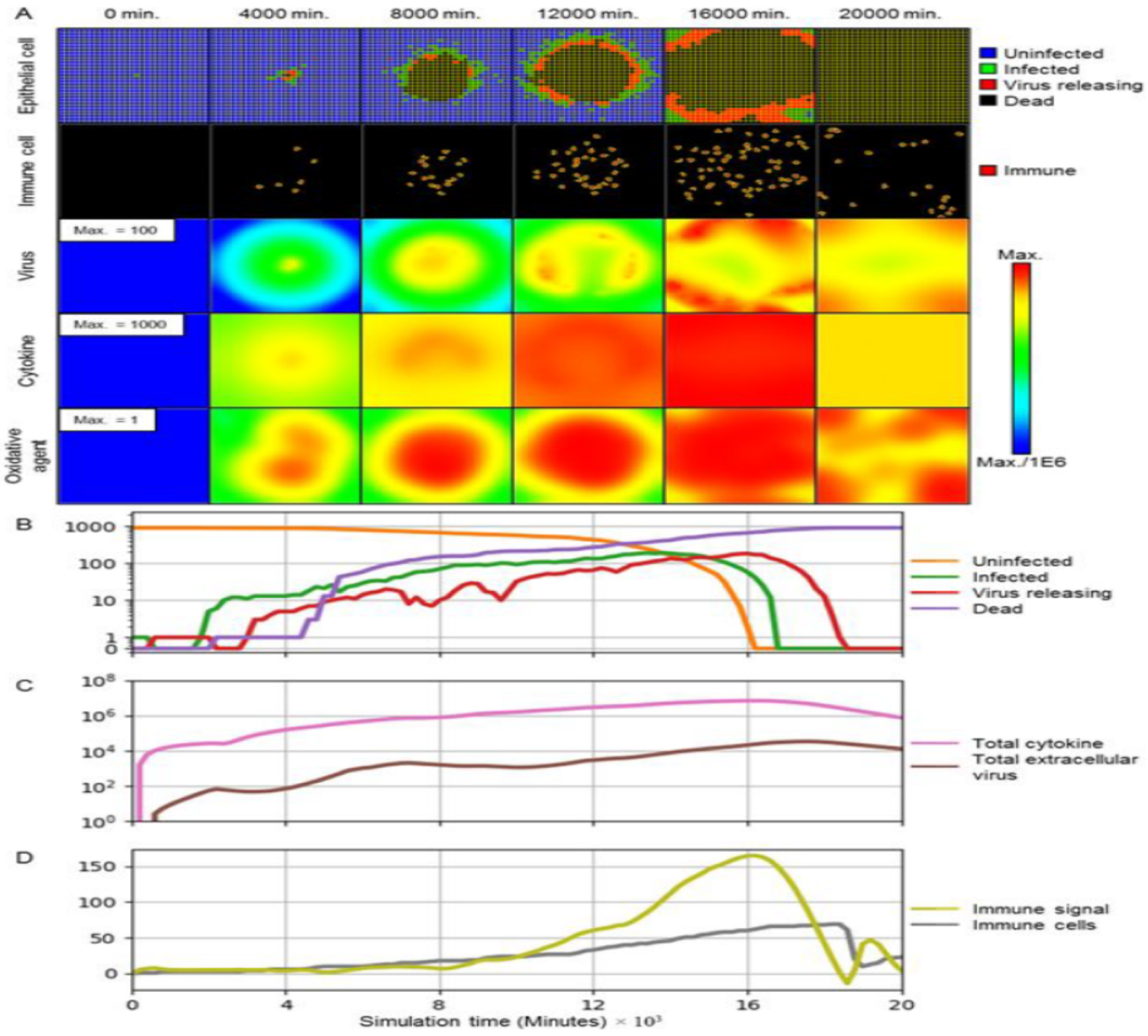


Figure 3. Simulation of the progression of infection in a patch of epithelial tissue of size 360 µm x 360 µm starting from a single infected cell for a representative simulation using the baseline parameters given in Table 1. A. Snapshots of spatial configuration *vs* time, showing progression of a simulated 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

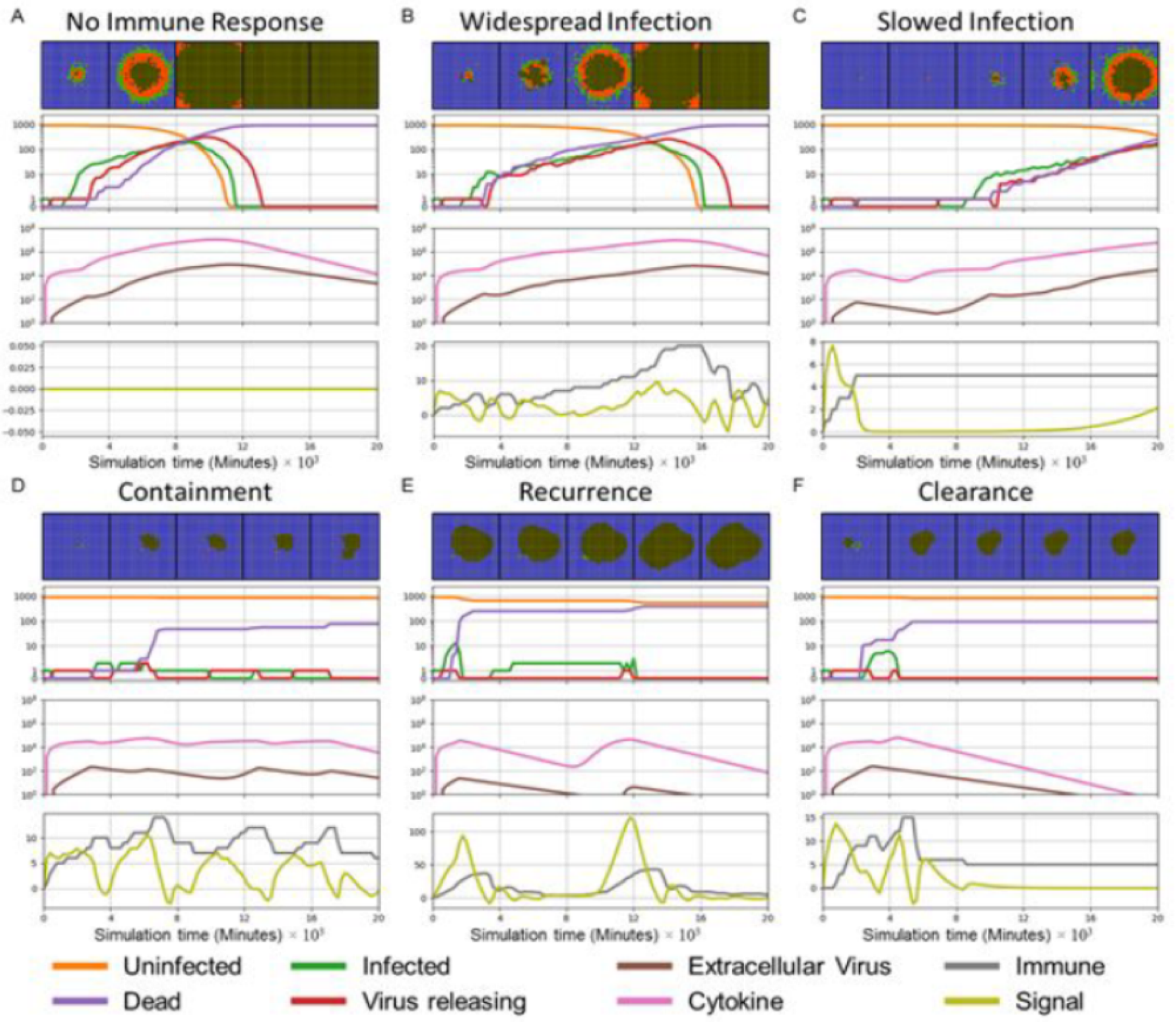


Figure 4. Patterns (classes) of spatiotemporal infection dynamics. First row: snapshots of spatial configurations of the epithelial cells. Color coded: uninfected (blue), infected (green), virus releasing (red), dead (black). Times from

Example of the Application of CompuCell3D

A multiscale model of viral infection in epithelial tissues

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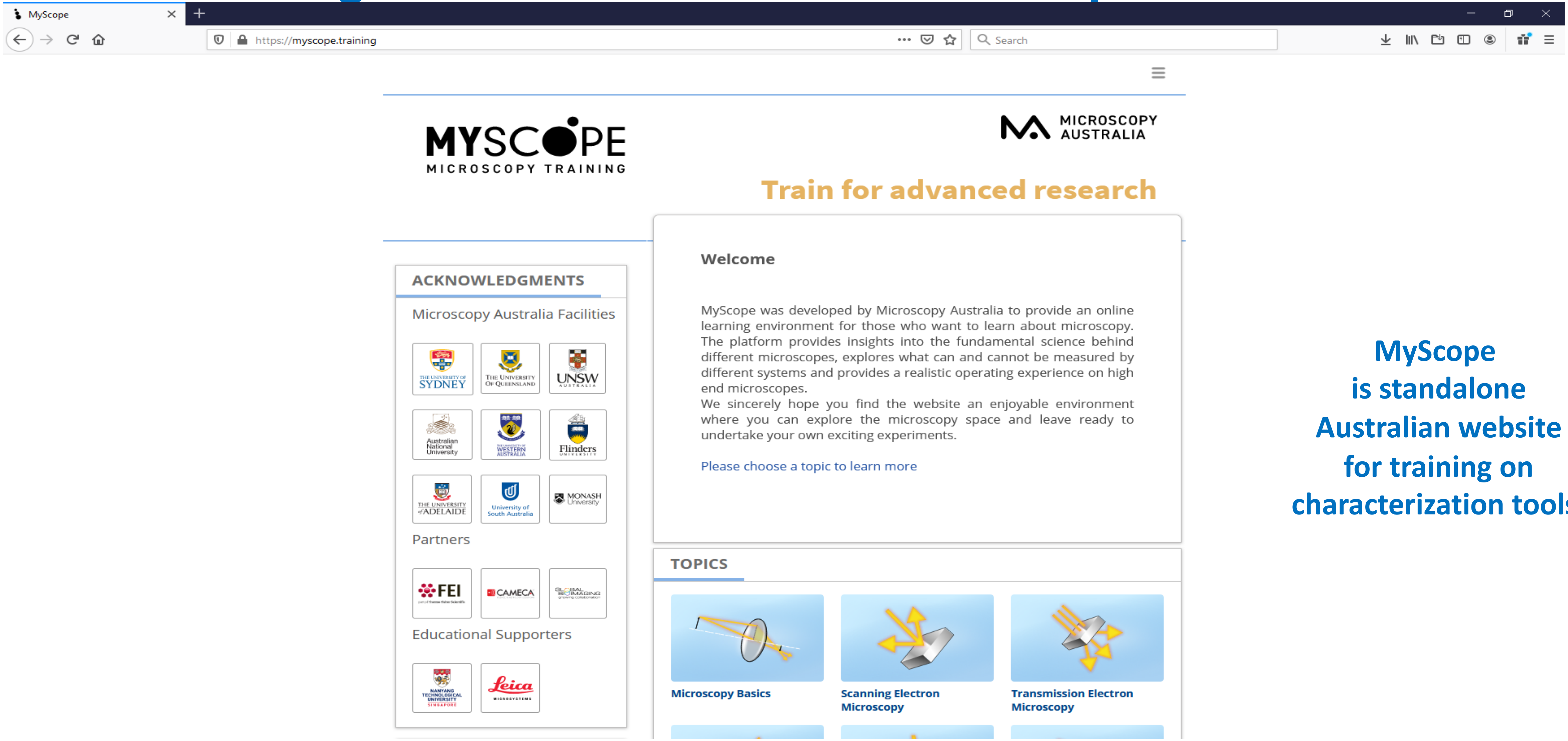
Another Online Resource:
A great characterization virtual experience:



MyScope is standalone Australian website for training on characterization tools.

Conclusion

- Online visualization and simulation tools helps to enhance teaching/learning of nanoscale phenomena in Physics, Chemistry, Engineering, Engineering Technology, Molecular Biology, and Microbiology.
- Online learning supports STEM and Nanotechnology workforce development.
- RAIN provides free online remote access to real world Nanotechnology tools from the ease of classrooms, or home computers, across the country.
- RAIN visualization tools can be used to detect viruses.
- AFM is an inexpensive and portable promising tool for detecting viruses.
- NanoHub is an excellent simulation platform for introducing and analyzing nanotechnology phenomena at all educational levels at no cost.
- NanoHub's CompuCell3D simulation tool allows online simulation of COVID-19 without requiring any installations or downloads.
- CompuCell3D is a flexible scriptable modeling environment, which allows the rapid simulations for cancer, viruses, developmental biology, evolution, the immune system, tissue engineering, toxicology, and non-cellular soft materials.

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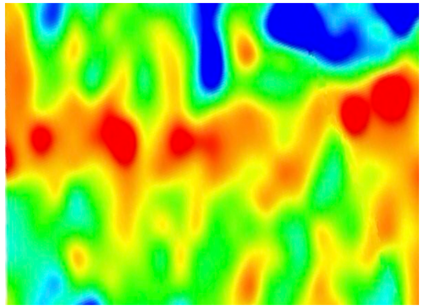
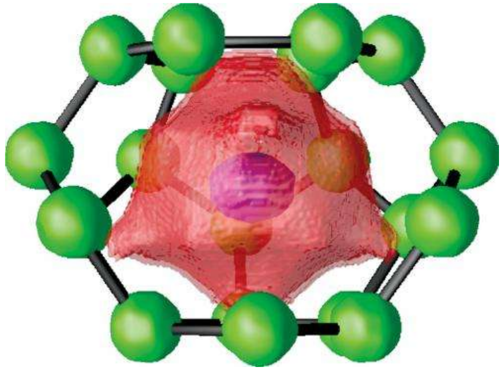


Online Visualization and Simulation Tools for Teaching Nanotechnology



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A detailed version of this presentation is available at HI-TEC Conference Website.

MNT Education Special Interest Group (MNT^{e}SIG Live) 2020 Virtual Conference Via Zoom July 27-28, 2020

Thanks for watching this presentation….Any Comments…Questions? 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