MNT-EC nanoHUB Presentation March 16, 2021 Handout
Feel free to contact me with any questions: Tanya (nanohub.engagement@gmail.com)

nanoHUB

Relevant Groups
- **nanoHUB Beginners**
- **Group: Nanotechnology Workforce Development**
- **MNT Educator Community**
- **Chemistry ~ Simulation Tools**

Tools and Related Resources

***ab initio* simulations with ORCA** **https://nanohub.org/tools/orcatool**

CNT Bands https://nanohub.org/tools/cntbands-ext
- CNT Band worksheet

Crystal Viewer version 2.3.4 Crystal Viewer Tool
- Quick and Easy Guide to Carbon Structure Simulations using Crystal Viewer Tool
- Using nanoHUB to Introduce Elementary and Middle School Students to Models and Simulations

Crystal Viewer version 3 Crystal Viewer Tool
- nanoHUB Simulation Activity - Orientations of Common Single Crystal Substrates
- How to View (100), (110) and (111) Planes in Silicon Using Crystal Viewer 3.0
- How to View Atomic Planes in FCC, NaCl and Simple Cubic Structures using Crystal Viewer

Stanford Stratified Structure Solver https://nanohub.org/tools/s4sim
- Resources: Exploring Thin Film Interference Colors through Simulation

Process Lab: Oxidation https://nanohub.org/resources/prolabox
- Exploration of the Oxidation Rate of Silicon Wafers via Simulation

Protein Contact Maps https://nanohub.org/tools/contactmaps

Jupyter Notebooks in your Personal nanoHUB Filespace

Jupyter Notebook https://nanohub.org/tools/jupyter Anaconda 6.0 (Octave, Python, R)

Jupyter Notebook with anaconda 5.1 https://nanohub.org/tools/jupyter51 (MatLab, Octave, Python, R)
- Setting up Your nanoHUB File Structure in Jupyter Notebooks

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This document is available at: https://tinyurl.com/nH2021Mar16

Published Jupyter Notebooks
("Read Only"; you can save a copy to your personal nanoHUB filespace)

Data Analysis of Normal Data Sets in Engineering https://nanohub.org/resources/engdata

Illustrative Mathematical Concepts https://nanohub.org/resources/illustmath

Matlab Data Analysis Using Jupyter Notebooks https://nanohub.org/resources/matlabdata

- Teaching Engineering using Jupyter Notebooks https://nanohub.org/resources/33971

Demo of Loading and Visualizing Proteins from the RCSB Protein Data Bank https://nanohub.org/tools/proteindemo

ECG Data Analysis Using Machine Learning https://nanohub.org/resources/ml4ecg

Machine Learning for Materials Science: Part 1 https://nanohub.org/resources/mseml

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Other nanoHUB Resources
Enhancing your Micro and Nano Technology Courses with Free nanoHUB Resources and Simulations
- Presentation slides

"Turning Fruit Juice into Graphene Quantum Dots" Supplementary Lesson Plans: Going Atomic
- Adds nanoHUB simulation activities to this NNCI activity

Examples of Documentation and Tutorials for Jupyter packages

Mendeleev Plotting (Periodic Table)
https://mendeleev.readthedocs.io/en/stable/notebooks/03_plotting.html

BioPython
https://biopython.org/
Tutorial:
http://biopython.org/DIST/docs/tutorial/Tutorial.html#sec9

This document is available at: https://tinyurl.com/nH2021Mar16