Issue 56

Stay informed about what's happening on nanoHUB! Check out our featured resources, upcoming webinar series and more, below.

Back to School Webinar Series

This series of webinars will give you the opportunity to learn from faculty who use nanoHUB in their classes and research. Faculty will share how they use nanoHUB simulation apps and assignments, as well as share aspects of teaching or doing research using nanoHUB resources. There will be time for live Q&A during each session. Registration and online compute resources are free of charge.

It's not too late to implement nanoHUB into Fall courses! Faculty who are interested can request support from the nanoHUB team. Please reach out via our *Contact Us form*.

Hands-on Teaching with Jupyter Notebooks in nanoHUB

In the first session, "Hands-on Teaching with Jupyter Notebooks on nanoHUB", Prof. Michael Reppert will share how he uses nanoHUB in his college chemistry courses at Purdue University. The ideas and techniques are also applicable to fields other than chemistry.

Date and time
Tuesday, September 6, 2022 from 1:00 - 2:00 PM EDT

Register here

Teaching electronic structure methods in chemistry using simulation tools in nanoHUB

Join Prof. Nicole Adelstein for "Teaching electronic structure methods in chemistry using simulation tools in nanoHUB." Prof. Aldestein will share how she uses nanoHUB to teach her upper-division chemistry students at San Francisco State University.

Date and time
Wednesday, September 7, 2022 from 1:00 - 2:00 PM EDT

Register here

Introduction to computational chemistry using the NUITNS simulation toolkit in nanoHUB

In the session, "Introduction to computational chemistry using the **NUITNS simulation toolkit** in nanoHUB," Prof. Tomekia Simeon will share how she uses nanoHUB's free online simulation resources in her course.

Date and time
Friday, September 9, 2022 from 1:00 - 2:00 PM EDT

Register here

Data Cleaning with MATLAB

In "Data Cleaning with MATLAB," Dr. Kelsey Joy Rodgers will share how to simplify and automate your data cleaning tasks with **MATLAB on nanoHUB**.

Date and time
Monday, September 12, 2022 from 1:00 - 2:00 PM EDT

Register here

Introduction to Machine Learning for materials science

This session is a set of back-to-back machine learning workshops with Drs. Benjamin Afflerbach and Ryan Jacobs. Part I is an introduction to **Machine Learning for Materials Science** that is appropriate for people with no prior experience who would like to start teaching machine learning concepts. Part II is a more advanced, complementary training with the **Materials Simulation Toolkit for Machine Learning (MAST-ML)**. The workshops form a series, but you are welcome to join just one if you'd like.

Date and time
Tuesday, September 13, 2022 from 1:00 - 2:00 PM EDT

Register here

Introduction to DFT simulations in nanoHUB

In this session, Prof. André Schleife of University of Illinois at Urbana-Champaign will give an introduction to DFT simulations in nanoHUB.

Date and time
Wednesday, October 5, 2022 from 1:30 - 2:45 PM EDT

Register here

HUBzero® Platform News

Hubzero® Reaches 20 Year Anniversary

The year 2022 marks the 20 year anniversary of the **Hubzero project**. Initiated as nanoHUB.org by Professor Mark Lundstrom, the inaugural Director of the Network for Computational Nanotechnology (NCN) in 2002 at Purdue University, Hubzero has demonstrated staying power beyond that of most academic projects. As nanoHUB.org realized success, others saw this success and suggested that its science gateway cyberinfrastructure should be made available to others in need of a science gateway. Under the guidance of Professor Gerhard Klimeck, the current Director of NCN at Purdue, and Michael McLennan, the founding Hubzero director, the team undertook an effort to abstract the underlying Cyberinfrastructure from the nano content to go beyond nanoHUB.org, and Hubzero was born. Today, Hubzero has been used to construct over 70 science gateways serving a wide variety of scientific domains with a combined total of millions of unique users.

New Resources on nanoHUB

### Machine Learning Predicts Additive Manufacturing Part Quality: Tutorial on Support Vector Regression

In this **hands-on tutorial**, Davis McGregor demonstrates the use of machine learning to accurately predict defects in additive manufacturing (3D printing). You will learn how to train a support vector regression (SVR) model to predict the dimensions of AM parts based on the design geometry and manufacturing parameters.

You can **run the SVR Machine Learning tool here** as you work through the tutorial.

Microstructure Modeling with OOF2 and OOF3D

This resource is an **online tutorial on microstructure modeling** with the recently updated **OOF2** and **OOF3D** simulation tools. These tools are available to use for free on nanoHUB, without the need to download any software.

You can also join the new **OOF Users Group in nanoHUB**, where you can post questions in the group forum and discuss all things OOF with the nanoHUB OOF community, including the tutorial speakers (and OOF developers) from NIST.
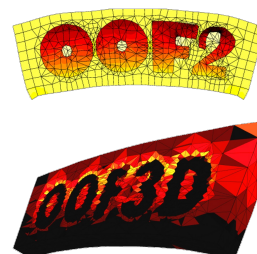
nanoHUB Tips and Tricks

nanoHUB Event Calendar

Did you know? nanoHUB hosts several online workshops and webinars throughout the year. You can view all upcoming events on the **nanoHUB Events Calendar**. To easily navigate to the events calendar, visit the nanoHUB homepage, find and hover over the *Community* tab in the top middle of the page, and click *Events*.

Check back often, as new events are being added each month.

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Do you have a suggestion or nanoHUB success story you'd like to share? Use our Contact Us form and you may see your submission in a future newsletter!

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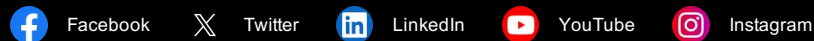
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