



Issue 63

Stay informed about what's happening on nanoHUB! Check out upcoming events, new resources, and more below.

Upcoming Events

Online Seminar: Chemistry & Materials with the Amsterdam Modeling Suite



In this online talk, [Dr. Nicolas Onofrio](#) will give an overview of the Amsterdam Modeling Suite (AMS) to perform atomistic simulations at various levels of theory. First, he will describe the AMS driver designed to explore potential energy surfaces of molecules and periodic systems, and its integration with AMS' DFT, DFTB and force field engines. To illustrate the capability of AMS' DFT engines, he will introduce a few studies performed with ADF and its periodic extension BAND. Second, he will focus on force fields (ReaxFF and MLPotential) to describe reactive systems and polymer chemistry. Finally, Dr. Onofrio will present PARAMS to create new force field parameters in order to describe novel molecular interactions. Along with this presentation, he will illustrate the various applications with short demos or videos performed with the AMS graphical user interface.

Date and time

Thursday, March 30 from 10:00 - 11:00 am EDT

This event has passed.

New Resources

Quantum Information Science -The 2022 Nobel Prize Backstory

In [this lecture](#), David D. Nolte, the Edward M. Purcell Distinguished Professor of Physics and Astronomy at Purdue University, gives the backstory to the 2022 Nobel Prize in Physics. Dr. Nolte presents a cast of characters starting with Einstein distrusting his own invention, David Bohm, a rare physicist exiled by the US government, and John Bell of CERN, who began his high-school education on a financial needs scholarship to a vocational school that included a class in brick laying. Learn the full story here: nanohub.org/resources/36928.

A Guided Tour of Interactive Jupyter Notebooks Powered by nanoHUB

In this [online presentation](#), Dr. Daniel Mejia will take you on a guided tour of interactive Jupyter Notebooks powered by nanoHUB. Jupyter is a powerful tool for data science and scientific computing that provides an intuitive interface for a variety of programming languages; Jupyter in nanoHUB provides even more features!

Gain a better understanding of Jupyter Notebooks, learn about new updates to Jupyter Notebooks in nanoHUB, and find out how to use libraries for data analysis and visualization. View the presentation here: nanohub.org/resources/36900.

Follow along in the Jupyter Notebook tool here: nanohub.org/tools/jupyter70
Find a guide to the new features here: nanohub.org/tools/jupyterguide70

Community News

Purdue Day of Giving

Save the date! Purdue University's annual Day of Giving takes place on **April 26, 2023**. Purdue Day of Giving is a 24 hour, online-based fundraising event in which people are encouraged to give back and help transform the various entities that make up Purdue University.

As a platform developed through the Network for Computational Nanotechnology (NCN) at Purdue University, nanoHUB is proud to participate in this day



of giving.

Consider supporting the sustainability of nanoHUB so we can continue to provide valuable educational resources to our users at no cost. **During the online donation process, select Network for Computational Nanotechnology/NanoHUB as the fund.** As we get closer to the event, we will share a direct donation link that includes the nanoHUB designation via email and our social media channels.

Learn more by visiting dayofgiving.purdue.edu.

Registration now open for next session of Schrödinger Online Courses

Through nanoHUB's partnership with [Schrödinger](#), you can level up your skill set with their hands-on, online computational chemistry courses at a discounted rate.



The next session of Schrodinger courses is now open for registration. The session runs from April 12 through May 24, 2023. Participants are able to work through the course material at their own pace during this timeframe.

Use code **NANOHUB6** to receive the special nanoHUB user discount. [Click here for full details and to register.](#) Please reach out to us via contact@nanoHUB.org if you have any questions.

2023 Multicell Virtual Tissue Modeling Online Summer School and Hackathon

Applications for the 2023 Multicell Virtual Tissue Modeling Online Workshop and Hackathon are now open! **Apply by June 1, 2023**, at the link below. Enrollment is limited and by application only. Registration is free.



Intro to Python: July 31, 2023
Introductory Course: August 1-4, 2023
Advanced Topics: August 7-11, 2023
Model-Building Hackathon: August 12-13, 2023

This year's workshop features an introductory course that teaches new users the basics of multicellular modeling using CompuCell3D, as well as an advanced topics course that covers a variety of high-level modeling options and features of CompuCell3D.

The CompuCell3D modeling environment allow researchers to rapidly build and execute complex Virtual Tissue simulations with minimal programming experience. CompuCell3D enables biological simulations from subcellular to tissue scales, supporting explicit cell shapes, cell migration, contact-mediated cell interactions, soluble signals, and complex cell state dynamics (gene regulatory, signaling, and metabolic networks). Try out some example models on nanoHUB without any installation: [CompuCell3D on nanoHUB](#).

Learn more and apply by visiting compuCell3d.org/Workshop23.

I-Corps Jumpstart: Nanotech and Advanced Materials - Great Lakes Region, Summer 2023

Are you interested in commercializing technologies from your nanotechnology or other advanced materials research? Do you have a great idea for a product or service but need help determining its commercial potential and the best path to commercialization? If so, the Nanotech and Advanced Materials Jumpstart Regional I-Corps Course might be for you!



This free program is designed to provide the training, resources, and mentorship necessary to accelerate the commercialization of your innovation. Based on the Lean Launchpad methodology taught at over 300 universities worldwide, participants will learn about customer discovery, business models, and market analysis, and will receive feedback and guidance from experienced mentors.

The course also offers a wide range of benefits, including eligibility for the NSF I-Corps National Teams program and a \$50,000 grant for qualifying technologies and teams, preparation for applying to Small Business Innovation Research (SBIR) or Small Business Technology Transfer programs, and the development of the entrepreneurial mindset and toolset necessary for success in academia, industry, startups, or government.

The course is for faculty, researchers, and students with Nanotechnology and Advanced Materials-related ideas or Intellectual Property and a strong interest in commercializing their technology. It is offered online over the course of six weeks, beginning May 12, 2023. Applications are now open. [Learn more and apply here.](#)

SGX3 Internship Opportunity at TACC

Our partners at SGX3 invite graduate students seeking hands-on work experience to apply to their Summer Internship opportunity at the Texas Advanced Computing Center (TACC). The internship program is open to students anywhere in the United States.



Eligible applicants include graduate students majoring in computer science or computer engineering (or related fields). The student will be funded by SGX3 to join the TACC science gateway team for the summer, working on live, impactful gateways.

Students can use the internship experience to receive credit through their college or university if their institution has an independent study class or internship credit program. On the application form, students should indicate their intent to use the internship to satisfy requirements for university credits. The course/program number (if applicable) and description will be requested, and paperwork will need to be processed at the beginning and end of the internship.

To learn more and apply, visit sciencegateways.org/internships. Please feel free to share this opportunity with anyone who may be interested.

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!

How can you support nanoHUB? Check out our [donation page](#) to learn more.

Follow us on social media:



Facebook



Twitter



LinkedIn



YouTube



Instagram

The [Network for Computational Nanotechnology](#) and [nanoHUB.org](#) are supported by the [National Science Foundation](#).

