Issue 72

Stay informed about what's happening in the nanoHUB community by exploring upcoming events, new resources, and community news.

Happy Holidays!

As another year draws to a close, we want to take a moment to thank you for being part of our community. We've had an incredible year, filled with exciting partnerships, engaging workshops, and many new resources.

We're grateful for your contributions to nanoHUB, whether you've shared your research, participated in events, or used our tools to advance your studies or work. Your passion for science and nanotechnology is what makes nanoHUB such a special platform.

As we head into the holiday season, we wish you all a time of peace, joy, and renewal. We look forward to seeing you again in the new year, ready to tackle new challenges and achieve new accomplishments.

In the meantime, be sure to check out upcoming events and new resources below.

Upcoming Events

Integrating Programming and Cheminformatics into the Molecular Science Curriculum: Resources from the Molecular Sciences Software Institute using nanoHUB

Date and time
Thursday, January 18, 2024; 12:00 - 1:00 PM EST

Presenter
Ashley Ringer McDonald, Ph.D., California Polytechnic State University-San Luis Obispo

This presentation will describe open-source curriculum from the Molecular Sciences Software Institute (the MolSSI) to teach programming and cheminformatics using nanoHUB. The MolSSI is an NSF-funded institute that aims to improve software, education, and training in the computational molecular sciences. MolSSI offers a wide range of educational resources that teach topics such as programming, best practices in software development, modular modeling, and cheminformatics, all in the context of computational molecular science and engineering. Faculty are welcome to adopt or adapt any of these resources for their courses. This presentation will describe MolSSI resources available on nanoHUB, particularly highlighting a cheminformatics module that has recently been published as a nanoHUB tool.

This event has passed

New on nanoHUB

Schrödinger Materials Science AutoQSAR for Machine Learning

Schrödinger's AutoQSAR for Machine Learning educational tool is now available on nanoHUB.

Schrödinger's Materials Science platform integrates predictive physics-based simulation

with machine learning techniques to accelerate materials design. Their iterative process is designed to accelerate evaluation and optimization of chemical matter in silico ahead of synthesis and characterization.

The AutoQSAR tool is for automated creation, validation and application of QSPR models following a best practices approach. The available tutorials demonstrate the use of AutoQSAR to build and rank order numerical QSPR models, visualize atomic contributions to property predictions and use these models to make predictions on new, unseen datasets.

To access the tool, you must follow the instructions to join the **Schrödinger Materials Science Group**.

You can also find the following Schrodinger webinars on nanoHUB:

- **Hands-On Workshop in nanoHUB: Machine Learning Models for Ionic Conductivity with Schrödinger's AutoQSAR**
- **Data-Driven Materials Innovation: where Machine Learning Meets Physics**

Quantum Science at Purdue Undergraduate Workshop

The **Quantum Science at Purdue (QSaP) workshop** recently hosted numerous Purdue undergraduates and visitors in an event that showcased the fascinating world of quantum science and technology.

You can now access **recordings of the workshop presentations in nanoHUB**. Topics include:

- Electronic Structure
- Quantum Computing and Quantum Information
- Quantum Dynamics and Open Quantum Systems
- Quantum Optics
- Quantum Materials

Each topic is presented as a module of three talks The topic is first introduced through a 40-minute talk targeted at the advanced undergraduate level and assuming minimal prior knowledge. These introductory talks are followed by two short "application" talks that illustrate how these concepts are at work in modern quantum science research applications.

NASA's Mars Helicopters - Past, Present and Future

On April 19, 2021, in the Jezero Crater on Mars, the Ingenuity rotorcraft performed the first powered flight on another planet marking a milestone in interplanetary exploration. Designed as a technology demonstrator and a secondary payload for NASA's Mars 2020 mission, its primary purpose was to prove that powered flight is possible in the extremely thin Martian atmosphere. While the mission/ flight wasn't intended for transportation but rather to test the concept of aerial exploration on Mars, Ingenuity's success paved the way for future missions to use helicopters and drones for scientific exploration, mapping, and reconnaissance on other planets by demonstrating the potential for aerial exploration on Mars.

In this presentation, Gregory Allen, a senior radiation effects engineer at the Jet Propulsion Laboratory, California Institute of Technology, celebrates Ingenuity's success, explores the path it took to get there, and looks at the future of autonomous flight on Mars.

nanoHUB Community News

Summer 2024 SGX3 Internship Experience

Austin, TX
Applications due January 31, 2024

The SGX3's Workforce Development team will offer a summer program aimed at graduate students. Eligible applicants include graduate students majoring in computer science or computer engineering (or related fields). The students will be funded by SGX3 to join the TACC science gateway team for the summer, working on live, impactful gateways. Each student will also receive impactful mentorship from TACC researchers and opportunities to grow their leadership skills. **Apply before January 31, 2024**.

Gateway Focus Week
Looking to build a sustainability plan for your science gateway? Planning to write your next funding proposal? Join SGX3 and SGCI at the next **Focus Week** to create your starter sustainability toolkit.

Gateway Focus Week is an intensive week-long workshop designed for innovative research teams to work together on producing a strong sustainability plan. You'll leave Focus Week with a clearer definition of your project's value, its audience, and its positioning in the competitive landscape along with tools you can use as your project continues to mature.

Focus Week 2024 takes place April 15-19, 2024 at the Texas Advanced Computing Center (TACC) in Austin, TX.

Apply via the **Focus Week Workshop Application**. The Focus Week **application will close on March 15, 2024**.

Thanks to the generous support of NSF, there are no workshop registration

fees. Attendees will only need to cover their travel, lodging, and meal costs.

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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