Issue 74

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

Upcoming Events

DFT with SIESTA, data visualization, and a sophomore-level CURE with the MIT Computational Nanoscience Toolkit

Date and time
Tuesday, March 19, 2024; 12 p.m. EDT

In this webinar, **Dr. David Strubbe** will discuss how he has been using the **MIT Atomic-Scale Modeling Toolkit** (which he co-developed) for a sophomore-level modern-physics class as well as an undergraduate/graduate condensed-matter physics class at the University of California, Merced. He will focus on use of the density-functional theory (DFT) code SIESTA and visualization code XCrySDen, for calculations of structure, density, and wavefunctions, and visualization of these quantities as well as of Brillouin zones and Fermi surfaces. He uses the toolkit for a Course-based Undergraduate Research Experience (CURE) in modern physics to illustrate ideas of the particle-in-a-box model via heterojunctions of 2D materials. The students generate new data about heterojunctions, assessing quantum confinement of wavefunctions and their potential suitability for quantum well optoelectronic devices.

Register here

### Purdue University Day of Giving

Purdue University's annual Day of Giving will be held on Wednesday, April 24, 2024. nanoHUB was developed through the Network for Computational Nanotechnology (NCN) which is based at Purdue University. You can **learn more here**.

Our goal is to raise funds to support the sustainability of nanoHUB and continue providing an open and free platform for computational research, education, and collaboration. Please consider giving a gift on April 24. Stay tuned for more information and for other ways to help make an impact on Purdue Day of Giving.

New on nanoHUB

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

In **this presentation**, **Dr. Ashley Ringer McDonald** of Cal Poly San Luis Obispo describes open-source curricula from the **Molecular Sciences Software Institute (the MolSSI)** to teach programming and cheminformatics using nanoHUB, particularly highlighting the **Python for Cheminformatics** tool published in nanoHUB. Faculty are welcome to adopt or adapt MolSSI resources for their courses.
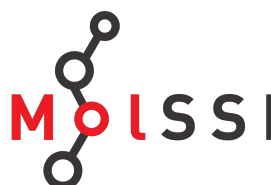
The Keys to Learning: Unlocking Your Brain's Potential

In this two-part presentation by **Prof. Michael R. Melloch** of Purdue Electrical and Computer Engineering, learn about the many things that influence learning. **Part I** covers neuroplasticity, memory, and effective learning techniques. **Part II** includes sleep, mindset, self-control and grit, exercise, meditation, and nutrition.

nanoHUB Community News

New MolSSI Faculty Development Program

Apply to the Molecular Sciences Software Institute (the MolSSI) professional development program by **Thursday, February 29, 2024**. The program provides financial support and training to help faculty integrate programming and computation in their curriculum. Learn more and **apply here**.

SGX3 Coding Institute

The SGX3 Coding Institute is focused on gateway development for undergraduate students at Elizabeth City State University. The workshop covers the core skills needed to be productive in the design and maintenance of science gateways.

The program is presented as short tutorials alternated with practical exercises, and all instruction is done via live coding.

The next SGX3 Virtual Coding Institute will take place June 3-27, 2024! Selected Participants receive a stipend of $2000. **Apply here by April 30, 2024**.

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.

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