Issue 70

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

Upcoming events

Machine Learning for Materials Science with Schrödinger

Date and Time
Tuesday, October 31, 2023 from 1 - 2 p.m. EDT

Machine learning (ML) has revolutionized materials science and chemistry with the help of deep learning innovations and the availability of larger and larger datasets. Many industrial scientists want to adopt a data-driven and AI-based design approach, but they face challenges with limited datasets and complex materials that need customized feature engineering. Furthermore, typical ML methods often struggle with interpretability and generalization to new chemical domains. In this webinar, we show how Schrödinger's tools can address these common issues by using a combination of physics-based simulation data, enterprise informatics, and chemistry-aware ML. We illustrate how this synergistic approach can transform materials innovation across a broad range of technology fields. Specifically, we will present case studies in the following areas:

- Using molecular dynamics simulations to generate features that improve the accuracy of ML models for viscosity predictions
- Building interpretable ML models to predict the ionic conductivity of Li-ion battery electrolytes
- Enhancing the performance of ML models for predicting properties such as absorption and emission wavelengths, fluorescence lifetime, and extinction coefficients of organic electronics using features derived from density functional theory

This integrated approach represents a new frontier in materials science and chemistry, combining the strengths of ML and physics-based methods.

Register here

Hands-On Workshop in nanoHUB: Machine Learning Models for Ionic Conductivity with Schrödinger's AutoQSAR

Date and Time
Tuesday, November 7, 2023 from 1 - 2 p.m. EST

We are in the midst of an inflection point in the utilization and impact of molecular modeling in materials science, particularly for industrial applications. This inflection is driven by significant advancements in compute power, methods development, and the integration of physics-based methods with machine learning.

In this workshop, we will demonstrate the hands-on use of Schrödinger's MS Maestro graphical user interface within nanoHUB to perform machine learning model creation and implementation.

In particular, we will walk participants through a hands-on demonstration of **Schrödinger's AutoQSAR tool** for predicting experimental ionic conductivity of ionic liquids. Note that while the example demonstrated here will be tailored towards energy materials, the same workflow can be applied for a variety of materials science applications, ranging from organic electronics to complex formulations.

In order to participate in the hands-on portion of the workshop, please be sure to request membership to the **Schrödinger Materials Science nanoHUB group** prior to the seminar. Otherwise, feel free to simply join the session and watch the demonstration.

Register here

nanoHUB Community News

Nanotechnology Infrastructure Leaders Summit

Last month, US leaders in nanotechnology met for the first ever Nanotechnology Infrastructure Leaders Summit in Washington D.C.

nanoHUB director, Dr. Gerhard Klimeck was in attendance along with other leaders of user facilities, open research laboratories, and innovation institutes to discuss creating a more seamless national network, streamlining the pipeline from discovery to commercialization.

Find a summary of the event **The White House Readout**.

New on nanoHUB

Recitation Series for Semiconductor Education (Fall 2023)

All seven sessions of our Fall 2023 Recitation Series for Semiconductor Education are now published in nanoHUB. You can find each of the recordings on **the series page**.

Each presentation focuses on one of the seven tools found within the **ABACUS Tool Suite** and includes several sample simulations and nanoHUB resources for the tool (including materials needed to easily integrate these resources into new and existing coursework).

An Introduction to Finite Element Analysis of Material Microstructure Properties in nanoHUB

This presentation includes a brief introduction to the fundamentals of FEA and OOF2, and demonstrates OOF2 simulations of stress distribution in example materials, with and without temperature effect.

The Department of Materials Science and Engineering at UIUC has incorporated several computational modules into undergraduate courses that use FEA to explore mechanical properties of materials, with the help of **OOF2 in nanoHUB**. Yang Dan shares his experience as an instructor in these courses on how OOF2 and nanoHUB facilitate teaching and learning.

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!