Issue 69

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

New on nanoHUB

Schrödinger Materials Science AutoQSAR for Machine Learning

Schrödinger's **AutoQSAR** for Machine Learning educational tool has recently been implemented in 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.

Various **tutorials** are available in nanoHUB to allow educational use of Schrödinger's AutoQSAR tool for materials science. 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 learn more by registering for Schrödinger's upcoming webinars in the *Upcoming Events* section above.

Recitation Series for Semiconductor Education (Fall 2023)

Thank you to everyone who attended our Recitation Series for Semiconductor Education. For those who were not able to attend or would like a refresher, you can find **the recordings** on nanoHUB. The remaining recordings will be published soon.

The objective of this recitation series is to enable faculty to enhance existing or new semiconductor classes with interactive simulations found in the **ABACUS Tool Suite**. Simulations and animations can immerse students into “what if” scenarios and engage them in more active forms of learning, including explorations used in homework assignments and design projects.

nanoHUB Community News

Science Gateways 2023 Conference - Registration Closing Soon!

Join the Science Gateways Community for their annual Gateways Conference, held Monday, October 30 - Wednesday, November 1, 2023 in Pittsburgh, PA.

The regular registration rate ($550) and student registration ($350) will close **Friday, October 6, 2023**. **Click here to register.**

Gateways 2023 is an opportunity for people working with science gateways to showcase their ability to teach, empower and engage research, and provide technologies to various communities. There will be diverse options for sharing work and networking. The format includes tutorial sessions, presentations, panels, posters, demos, and a BYOP - Bring Your Own Portal.

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!