Issue 73

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

Stay Up to Date with nanoHUB

Have you moved to a new organization in the last few years? Do you want to showcase your publications to the nanoHUB community? As we begin a new year, it's a great time to refresh your online presence by updating your nanoHUB profile.

Updating your nanoHUB profile is simple and only takes a few minutes. To do so, log in to your account, hover your cursor over “logged in” in the upper right corner of the page, and select “profile.” From there, you can update contact information such as your email address, as well as update your organization and position type.

You control what others see. You can keep personal information private, while publicly sharing your professional accomplishments by adding your ORCID ID, Google Scholar URL, ResearcherID, ScopusID, and ResearchGate ID.

Make sure to also enter your interests to receive future communications on events and materials that are relevant to you.

Keeping your profile up to date helps ensure you are receiving the latest information about nanoHUB news and activities. More detailed instructions on how to update your account are **available here**.

Upcoming Events

SGX3 Webinar: Science Gateways & FAIR

Date and time
Thursday, January 25, 2024; 3 PM EST

Join our partner, SGX3, for their upcoming webinar on Science Gateways & FAIR with presenters Sandra Gesing and nanoHUB Deputy Director Alejandro Strachan.

The FAIR (Findable, Accessible, Interoperable, and Reusable) principles have created significant momentum in the research community, recognizing a need to improve the quality of research by establishing common reproducibility standards.

Science gateways, like nanoHUB, provide an excellent opportunity to achieve FAIRness of research data and software while also bringing in a lot of complexity with the different layers of FAIRness: FAIRness of the science gateway framework, FAIRness of services, FAIRness of embedded data, to name a few.

Join the webinar to learn how nanoHUB has helped address challenges and offers measures to improve FAIRness. The webinar goes into details for FAIR and science gateways in general and especially for solutions in nanoHUB.

Register here

New on nanoHUB

Machine Learning for Materials Science with Schrödinger

In **this presentation**, principal scientist at Schrödinger, Anand Chandrasekaran, demonstrates how Schrödinger’s tools can address common challenges faced by scientists who want to adopt a data-driven and AI-based design approach by using a combination of physics-based simulation data, enterprise informatics, and chemistry-aware ML. He illustrates

how this synergistic approach can transform materials innovation across a broad range of technology fields.

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

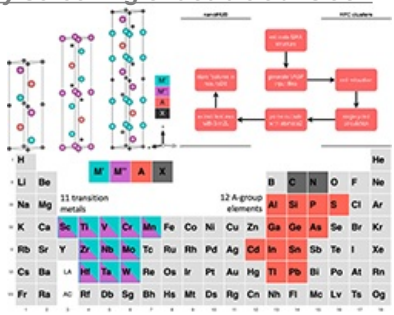
In **this workshop**, Dr. Michael Rauch demonstrates the hands-on use of Schrödinger's MS Maestro graphical user interface within nanoHUB to perform machine learning model creation and implementation. In particular, he walks through a hands-on demonstration of **Schrödinger's AutoQSAR tool** for predicting experimental ionic conductivity of ionic liquids. *Note that while the example demonstrated here is 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 access the tool please be sure to request membership to the **Schrödinger Materials Science Group**.

New Publications by Strachan Group Using nanoHUB Tools

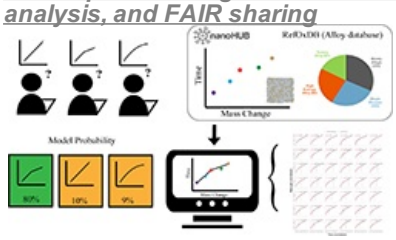
The **Strachan Group** led by nanoHUB Deputy Director Alejandro Strachan, has recently published two papers using nanoHUB tools. Learn more about each of the publications and tools:

High-throughput density functional theory screening of double transition metal MXene precursors



MXenes are an emerging class of 2D materials of interest in applications ranging from energy storage to electromagnetic shielding. MXenes are synthesized by selective etching of layered bulk MAX phases into sheets of 2D MXenes. Their chemical tunability has been significantly expanded with the successful synthesis of double transition metal MXenes. While knowledge of the structure and energetics of double transition metal MAX phases is critical to designing and optimizing new MXenes, only a small subset of these materials has been explored. The group presents a comprehensive dataset of key properties of MAX phases obtained using density functional theory within the generalized gradient approximation exchange-correlation functionals. Energetics and structure of 8,712 MAX phases have been calculated and stored in a queryable, **open database** hosted at nanoHUB. The tool in nanoHUB associated with the database of published results is **VASP ingestor**. It contains tools to query the database, and additional visualizations.

Mass uptake during oxidation of metallic alloys: literature data collection, analysis, and FAIR sharing



The area-normalized change of mass with time during the oxidation of metallic alloys is commonly used to assess oxidation resistance. Analyses of such data can also aid in evaluating underlying oxidation mechanisms. The group performed an exhaustive literature search and digitized normalized mass change vs. time data for 407 alloys. To maximize the impact of these and future mass uptake data, the group developed and published an open, online, computational workflow that fits the data to various models of oxidation kinetics, uses Bayesian statistics for model selection, and makes the raw data and model parameters available via a queryable database.

The tool, **Refractory Oxidation Database**, uses nanoHUB's Sim2Ls to make the workflow and data (including metadata) findable, accessible, interoperable, and reusable (FAIR). The group found that the models selected by the original authors do not match the most likely one according to the Bayesian information criterion (BIC) in 71% of the cases. Further, in 56% of the cases, the published model was not even in the top 3 models according to the BIC. These numbers were obtained assuming an experimental noise of 2.5% of the mass gain range, a smaller noise leads to more discrepancies. The **RefOxDB tool** is open access and researchers can add their own raw data (those to be included in future publications, as well as negative results) for analysis and to share their work with the community. Such consistent and systematic analysis of open, community-generated data can significantly accelerate the development of machine-learning models for oxidation behavior and assist in the understanding and improvement of oxidation resistance.

nanoHUB Community News

New MolSSI Faculty Development Program

The Molecular Sciences Software Institute (the MolSSI) is excited to announce a new faculty professional development program. The program provides financial support and training to help faculty integrate programming and computation in their curriculum. The application window opens on January 29

and closes on February 29. There will be an online information session about the program and the application process on Monday, January 29 at 1:00 pm ET. Learn more at **https://act-cms.molssi.org/#/home**.

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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