

[Elevating nanoHUB to the Next Level]



nanoHUB

53rd Midwest Theoretical Chemistry Conference at Purdue University

Agenda

- “What is nanoHUB?”
- Getting started in nanoHUB
- nanoHUB Chemistry resources

The screenshot shows the nanoHUB homepage with a dark blue header. The nanoHUB logo is on the left, and navigation links (EXPLORE, PUBLISH, COMMUNITY, ABOUT, SUPPORT) and user status (Logged in, Help, Search) are on the right. The main heading is "Making Data and Simulation Pervasive". Below this are four white tiles:

- Model & Simulate**: USE FOR RAPID EDUCATION AND RESEARCH. 500+ APPS, Tools, Most Popular. MORE
- Learn & Teach**: STRUCTURED, GLOBALLY USED RESOURCES. Simulation-Powered Curricula, Curated Education Materials, Courses, Lectures. MORE
- Develop Software**: ASSEMBLE YOUR OWN COMPONENTS. Jupyter, Linux Workstations, Engines / Frameworks, Machine Learning. MORE
- Share & Publish**: JOIN 3,000+ CONTRIBUTORS. Teaching Materials, Lectures, Tools / Apps. MORE

The screenshot shows the nanoHUB Chemistry group page. The header includes the nanoHUB logo, navigation links, and user status. The page title is "Chemistry". A blue banner reads: "Welcome to nanoHUB! We are a proud co-sponsor of the 53rd Midwest Theoretical Chemistry Conference. Access courses, simulations, and simulation-powered learning activities in nanoHUB, including over 7500 resources and 800 simulation tools." Below the banner, a link points to the "2023 Midwest Theoretical Chemistry Conference nanoHUB flier". A sidebar on the left lists navigation options: Overview, Getting Started, Courses, Chemistry Labs and Activities, Live Chemistry Webinars, Webinar Abstracts, Chemistry Simulations, K-12 Chemistry Outreach, Presentations, and Midwest Theoretical Chemistry Conference. The main content area includes a heading: "If you're new to nanoHUB, explore the tiles below to get started:" followed by three tiles: "Getting started on nanoHUB" (with a play button icon), "Browse live Chemistry webinars" (with a laptop icon), and "Chemistry Labs and Activities" (with a flask icon).

nanoHUB is an
open-access cyberinfrastructure

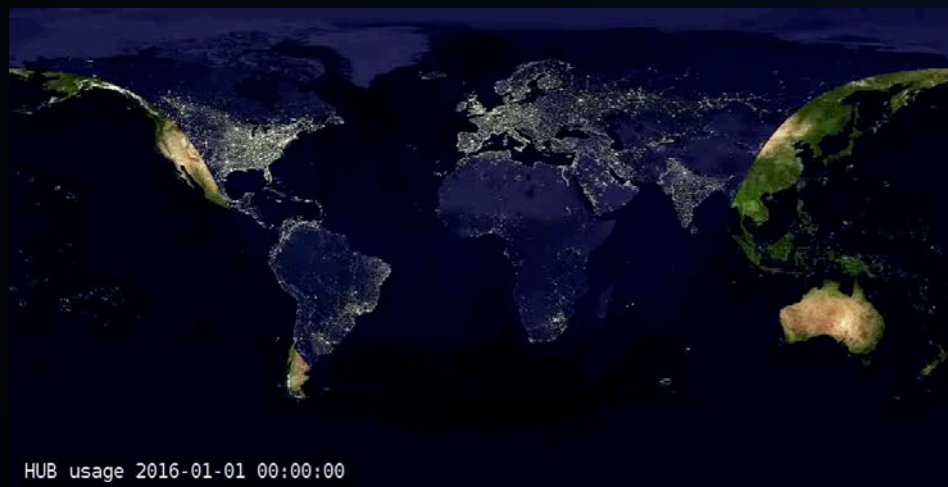
National Science Foundation
EEC 1227110

Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation



nanoHUB is...

- An app development workspace
- A toolbox of simulation apps
- A publishing platform
- A library of STEM resources
- A worldwide community



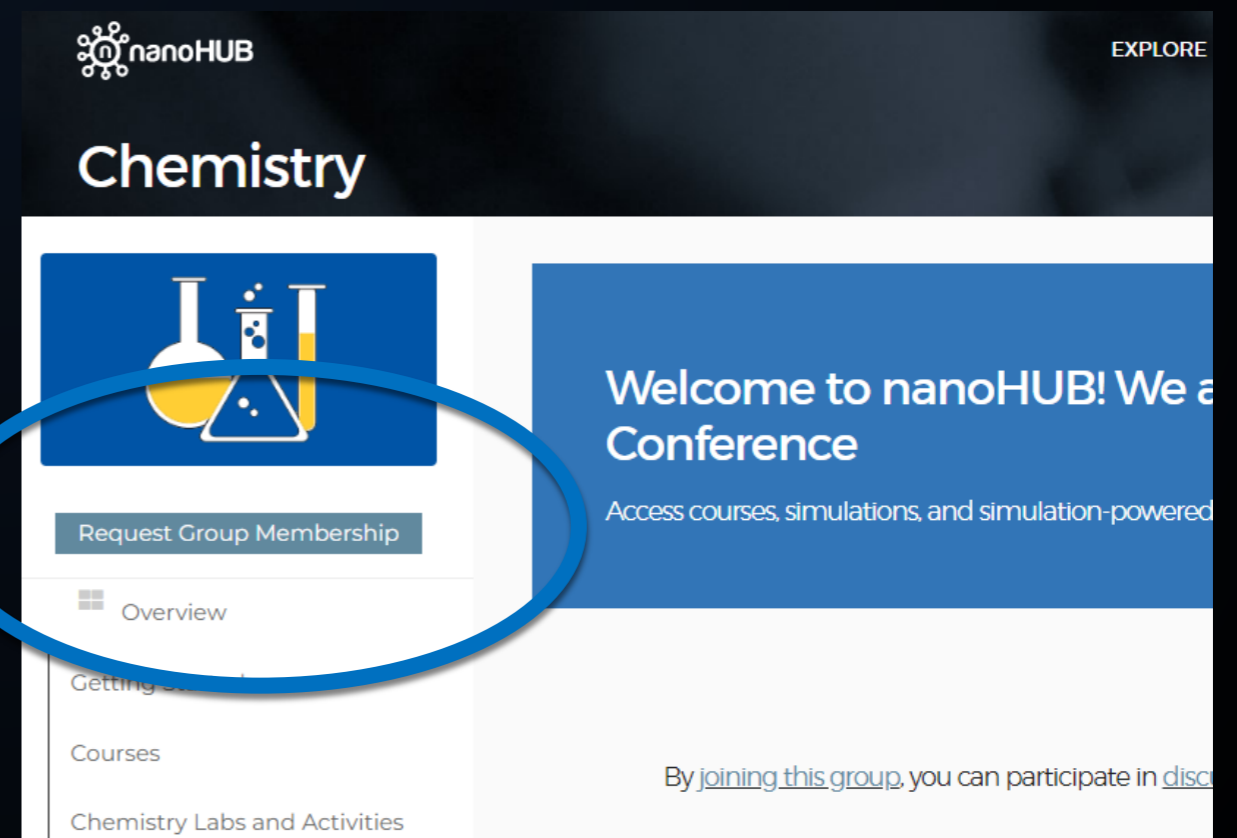
Getting started in nanoHUB

- Creating an account is FREE Visit [nanoHUB.org](https://nanohub.org)



The screenshot shows the nanoHUB homepage with a dark blue header. The navigation menu includes 'EXPLORE', 'PUBLISH', 'COMMUNITY', 'ABOUT', and 'SUPPORT'. On the right side of the header, the links 'Login', 'Sign Up', 'Help', and 'Search' are visible, with 'Login' and 'Sign Up' circled in blue. The main heading is 'Data and Simulation Pervasive'. Below this, there are three white boxes: 'Learn & Teach' (with sub-items: Simulation-Powered Curricula, Curated Education Materials, Courses, Lectures, MORE), 'Develop Software' (with sub-items: Jupyter, Linux Workstations, Engines / Frameworks, Machine Learning, MORE), and 'Share & Publish' (with sub-items: Teaching Materials, Lectures, Tools / Apps, MORE).

- A nanoHUB account allows you to access our Chemistry resources and simulation tools
- Join the nanoHUB Chemistry community here:
<https://nanohub.org/groups/chemistry/mwtcc>



The screenshot shows the nanoHUB Chemistry group page. The header includes the nanoHUB logo and 'EXPLORE'. The main heading is 'Chemistry'. Below this is a blue banner with a chemistry icon (flasks and test tubes) and a 'Request Group Membership' button, which is circled in blue. To the right of the banner is a 'Welcome to nanoHUB! We are having a Chemistry Conference' message. Below the banner is a sidebar menu with 'Overview', 'Getting Started', 'Courses', and 'Chemistry Labs and Activities'. The main content area below the banner contains the text 'Access courses, simulations, and simulation-powered...' and 'By joining this group, you can participate in disc...'



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Overview

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Getting Started

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Live Chemistry Webinars

Webinar Abstracts

Chemistry Simulations

K-12 Chemistry Outreach

Presentations

Midwest Theoretical Chemistry Conference

Members



Announcements



Collections

Welcome to nanoHUB! We are a proud co-sponsor of the 53rd Midwest Theoretical Chemistry Conference

Access courses, simulations, and simulation-powered learning activities in nanoHUB, including over 7500 resources and 800 simulation tools

[2023 Midwest Theoretical Chemistry Conference nanoHUB flier](#)

By [joining this group](#), you can participate in [discussions](#) on topics of interest to you and receive notifications about new Chemistry-related materials and events hosted by nanoHUB.

If you're new to nanoHUB, explore the tiles below to get started:



Getting started on nanoHUB



Browse live Chemistry webinars



Chemistry Labs and Activities





nanoHUB is an open and free online platform for computational education, research, and collaboration




Join our growing Chemistry community in nanoHUB!

nanohub.org/groups/chem/mwtcc

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- Run Computational Chemistry Simulations**
Run a wide range of computational chemistry simulations or perform data analysis and visualization using Jupyter Notebooks or MATLAB.
All tools run in nanoHUB and do not require download or installation.
- Build Custom Simulation Tools**
nanoHUB custom-built GUIs can support complex research workflows and make computational chemistry codes more accessible to students.
Connect to nanoHUB HPC resources, or your own.
- Connect to online databases**
 - RCSB Protein Databank
 - Crystallography Open Database
 - Materials Project
 - And more!You can easily request additional data connections.
- Increase the Impact of your Work**
Use nanoHUB's do-it-yourself publishing platform to publish your chemistry research and educational materials, and new simulation tools.
- Undergraduate and Graduate Level Chemistry Education**
Find tutorials, activities, full courses, seminars, and more!
- K-12 Outreach**
Find and share new K12 content for chemistry outreach.

Let us know what YOU would like to do in nanoHUB
Visit <https://tinyurl.com/nanohubmwtcc> or scan: 

Selected packages and tools installed in nanoHUB include:



Additional open source tools can be installed or updated upon request.

Please email contact@nanohub.org with any questions about nanoHUB.

nanoHUB is funded by the National Science Foundation: Award EEC-1227110, Network for Computational Nanotechnology Cyberplatform.



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Browse live Chemistry webinars



Chemistry Labs and Activities



Simulation Tools



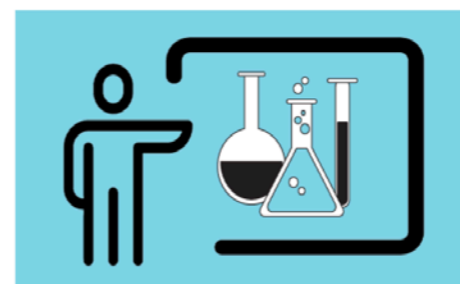
K-12 Chemistry Outreach




Presentations



Chemistry Forum



For Chemistry Instructors


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Chemistry Simulations

This page lists some of the simulation tools and apps relevant for chemistry.

You can view a list of all of the over 600 apps in the tools module in your nanoHUB dashboard.

nanoHUB Simulation Apps and Simulation Tool Engines

nanoHUB simulation apps have graphical user interfaces (GUIs) that make them easier to use than many traditional computational codes. nanoHUB apps provide valid default values, so that you can just click the launch button to see what the app does, and then you can return to the inputs to vary them and explore. Many apps also include examples that you can learn from.

Key benefits to running nanoHUB apps are that:

- The computational power is provided by nanoHUB. Depending on the app, these are provided by servers or supercomputer clusters.
- Apps run via a web browser, and they are OS agnostic (Mac, Windows, Linux are all OK!)
- No downloading or installation of code is involved
- You can run apps from a laptop, tablet or even a smart phone

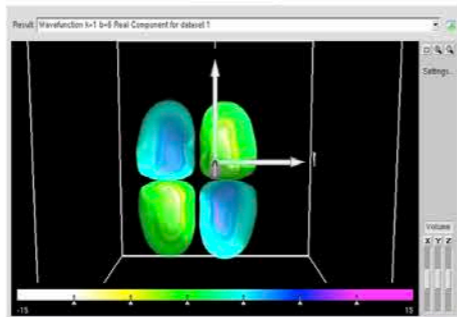
Each free nanoHUB account comes with 10 GB of free storage space, and three app sessions can be run simultaneously. Each session can have many runs, and persist over multiple days so long as you remain active with them.

Simulation "Tool Engines" are the computational codes that are installed in nanoHUB, and that the simulation apps connect to. Simulation apps in nanoHUB are built and published by the community and can be used by people around the world. Multiple simulation apps can be built on a single tool engine, and are often customized for a specific set of problems. If you don't find a simulation app that fits your needs, you are welcome to build and publish a new one! See the [Why Publish](#) page for more information, or submit a ticket in the help system describing what you want to do, and someone will help you. You can also build an app that connects to your own supercomputer cluster allocation.

Jupyter Notebooks, Sim2Ls and MATLAB

Chemistry Simulation Tools

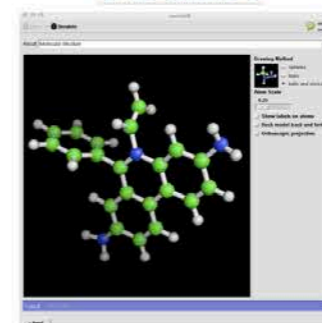
ABINIT



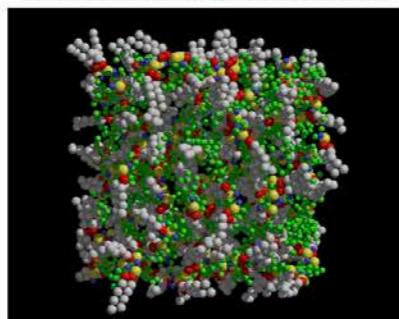
ab initio simulations with ORCA



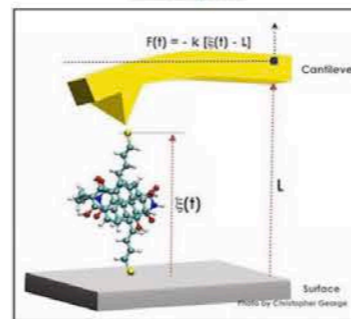
CNDO/INDO



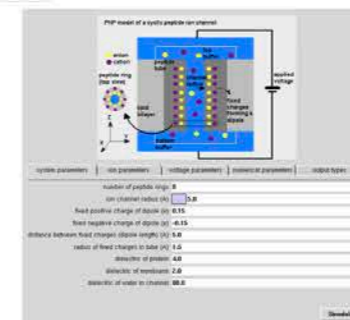
Coarse Grain Lipid Simulator



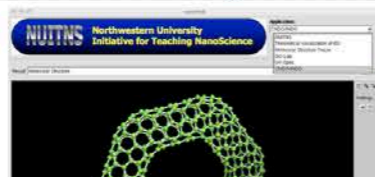
MOLpull



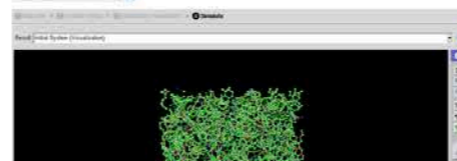
NP Cyclic Peptide Ion Channel Model



NUITNS: Northwestern University Initiative for Teaching Nanoscience



nuSIMM: nanoHUB user Simulation Interface for Molecular Modeling



Photosynthetic Protein Spectroscopy Lab



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Getting started on nanoHUB



Browse live Chemistry webinars



Chemistry Labs and Activities



Simulation Tools



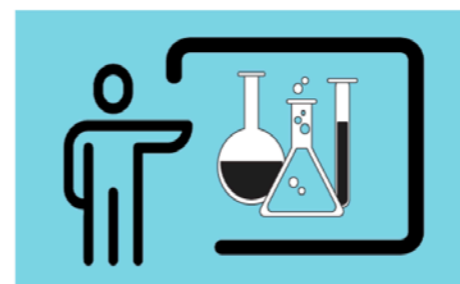
K-12 Chemistry Outreach



Presentations



Chemistry Forum



For Chemistry Instructors

Chemistry

DISCOVERABILITY: VISIBLE

JOIN POLICY: RESTRICTED

CREATED: 06 OCT 2013



Group Member

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MWTCC 2023 MEETING

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CHEMISTRY GROUP FORUM

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	Discussions	Posts
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Here is a place where you can share something about yourself with other group members. - Where do you work? - Do you teach? what level/ topics? - What are your research areas? - Anything else interesting.	Discussions	Posts
Questions	0	0
	Discussions	Posts

WEBINAR Q&A

2022-09-06 Webinar: Hands-on Teaching with Jupyter Notebooks on nanoHUB	0	0
If your questions for Dr. Reppert were not answered during the live webinar, you can post them here. Click the button to start a New Discussion.	Discussions	Posts
2022-09-07 Webinar: Teaching electronic structure methods in chemistry using simulation tools in nanoHUB	0	0
If your questions for Dr. Adelstein were not answered during the live webinar, you can post them here. Click the button to start a New Discussion.	Discussions	Posts

Statistics

Categories	12
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<http://biomolviz.org>: Biomolecular Visualization Literacy

Roderico Acevedo

10:45 am 03 Aug 2022

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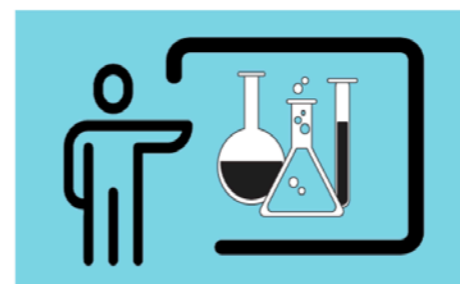
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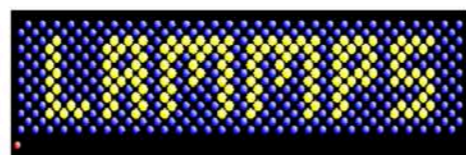


Chemistry Forum



For Chemistry Instructors

Explore selected tool engines and associated resources (including presentations, teaching materials, and more!) in nanoHUB:



LAMMPS



GAMESS



GROMACS



ORCA



Jupyter Notebooks

Learn about other topics in the [nanoHUB Education Center](#)



Education Center

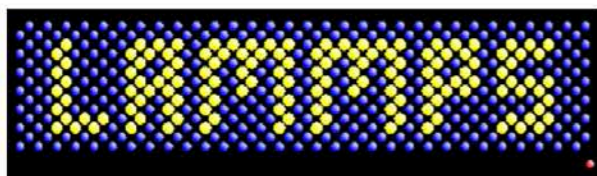
Tags: LAMMPS

More tags

LAMMPS

Search

Description



LAMMPS, Large-scale Atomic/Molecular Massively Parallel Simulator, is a classical molecular dynamics code with a focus on materials modeling.

LAMMPS has potentials for solid-state materials (metals, semiconductors) and soft matter (biomolecules, polymers) and coarse-grained or mesoscopic systems. It can be used to model atoms or, more generically, as a parallel particle simulator at the atomic, meso, or continuum scale.

[Launch LAMMPS tool](#)
[LAMMPS website](#)

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Note: Results do not include pending, unpublished, and some private items.

↓ Date ↓ Title/Name

Resources (1-20 of 51)

[Teaching and Learning with the MIT Atomic Scale Modeling Toolkit's Classical and Quantum Atomic Modeling Applications](#)

23 Dec 2022 Contributor(s): [Enrique Guerrero](#)

We will perform molecular dynamics computations using LAMMPS, simple Monte Carlo simulations including the Ising model, and run quantum chemistry and density functional theory computations.

[LAMMPS Data File Generator Tool Demo](#)

15 Apr 2022 Contributor(s): [Carlos Miguel Patiño](#)

A quick demonstration of the nanoHUB tool LAMMPS Data-File Generator. This was developed as part of the 2017 NCN URE program.



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