

Setting up a nanoHUB account and generating API key for citrination



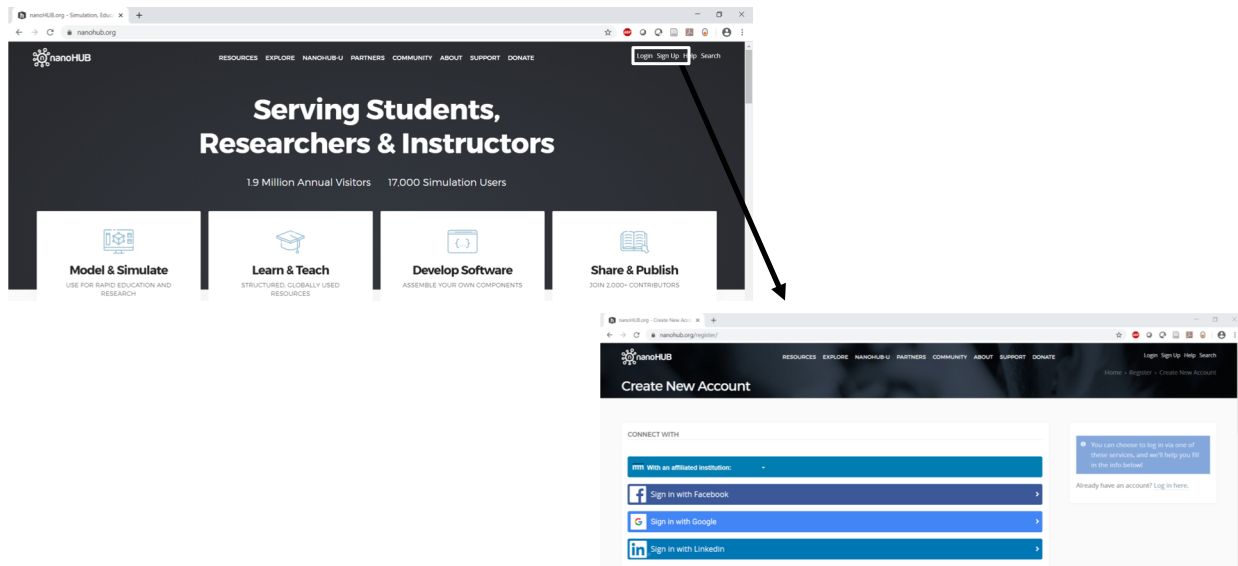
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STEP 1: Signing up for a nanoHUB account



STEP 2: Launch the matdatarepo tool in nanoHUB

From your browser go to link: <https://nanohub.org/tools/matdatarepo/>

Querying Data Repositories

By Zachary D McClure¹, Alejandro Strachan¹

¹. Purdue University

Query database repositories using Python based APIs and tips for managing data

Edit

Launch Tool

Version 1.0 - published on 03 Apr 2020

doi:10.21981/BJF0-9A31 [cite this](#)

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Click on Launch Tool to begin



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STEP 3: Navigating the landing page

- Read through overview
- Navigate to “*Introduction to materials databases and their accessibility*” **first**
- This will provide you information on how to get access to each of these repositories

Introduction to Data Science for Materials Science & Engineering

nanohub notebook by: Zachary D. McClure and Alejandro Strachan: Materials Engineering, Purdue University

The notebooks will be used to teach the basics of database querying and organization across three different API platforms.

Materials Project database access based on work published by: [Shuai Zhuo One et al.](#)

This Materials Project

Clone database access: [Citritone](#)

CITRINE

WolframAlpha API access: [WolframAlpha](#)

Overview

The following Jupyter Notebooks use API (Application Programming Interface) by Materials Project, Citritone, and WolframAlpha for materials design. Users can use the notebooks to learn about various querying APIs, and how they can be used to access large databases in the materials community. Notebooks are organized with instructions for accessing API keys for each application, and then performing queries with each API.

- #### Notebooks
1. [Introduction to materials databases and their accessibility:](#)
 - Introduction to materials databases and their accessibility
 - Collecting API keys for different platforms
 2. [Miscellaneous querying:](#)
 - Use Citritone API for database querying and learn how to upload your datasets
 - Example of other database queries using WolframAlpha
 3. [Querying and Managing Data from Materials Project:](#)
 - Perform large queries of Materials Project database for stable oxide structures
 - Manage data using Pandas dataframe and quickly access points of interest
 4. [Querying and Plotting Phase Diagram data for material compounds:](#)
 - Query Materials Project with element combinations and find stable phases
 - Organize data into accessible formats (dictionaries/Pandas) and plot phase diagrams from DFT calculations



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STEP 4: get API keys for Citrination

Keep your API key private! They are linked to your personal accounts and should not be distributed freely. Account access may be revoked by client if terms of use are broken.

Notebooks

[Introduction to materials databases and their accessibility](#)

- Introduction to materials databases and their accessibility
- Collecting API keys for different platforms

Miscellaneous querying:

- Use Citrination API for database querying and learn how to upload your datasets
- Example of other database queries using WolframAlpha

Querying and Managing Data from Materials Project:

- Perform large queries of Materials Project database for stable oxide structures
- Manage data using Pandas dataframe and quickly access points of interest

Querying and Plotting Phase Diagram data for material compounds:

- Query Materials Project with element combinations and find stable phases
- Organize data into accessible formats (dictionaries/Pandas) and plot phase diagrams from DFT calculations

Follow the links included in steps 3.2 to get your API key

3. Collection of API keys across platforms

3.1 Materials Project

Follow link provided to access login information at [Materials Project](#).

Create an account and find your API key under the API keys information section.



3.2 Citrination

Create an account at [Citrination](#). Your API key is listed in "Account Settings".

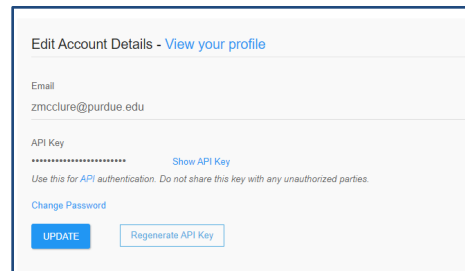
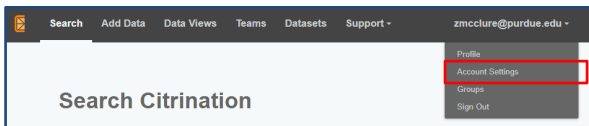


3.3 WolframAlpha

Create an account at [WolframAlpha](#). Request an AppID (API key) in the upper right corner after you login.



Citrination



- Create Citrination Account
- Under Account settings you will find your key