

Other Databases

Contents

- *Materials Platform for Data Science (MPDS)*
- *The Novel Materials Discovery (NOMAD) Repository*

1 Materials Platform for Data Science (MPDS)

The **Materials Platform for Data Science** (MPDS) is a high-quality database and provides instant access to a comprehensive repository of phase diagrams, crystal structures, physical properties and the corresponding literature references for inorganic materials. MPDS is the online edition of the full **Linus Pauling File** (LPF), the most authoritative database of property information for inorganic materials available today.

MPDS includes:

- more than 65,000 phase diagrams
- more than 350,000 crystal structures
- more than 620,000 property values

All derived from and referenced to over 250,000 scientific publications and the database is extended continuously.

Within MPDS it is possible to

- screen large numbers of design options for materials to focus experiment
- save resources and maximize your productivity with rapid and convenient access to relevant data
- conveniently find experimental data to validate computational approaches
- create your own data-centric solutions using the MPDS Application Programmer Interface (API).

Screen the scientific literature and reported property information for any desired inorganic material in seconds. You can view phase stabilities, access densities, thermal conductivities, (and a multitude of other physical properties), and scan crystallographic literature very swiftly. MPDS will save you hours of literature research and allow you to be confident that you have surveyed the range of experimental observation for your target materials. And you can export structures and employ them as the starting point for calculations in the leading materials atomistic simulation environment, *MedeA*.

A trial access to the MPDS [web site](#) [1] is possible via the menu sequence **File >> Visit MPDS web site** in the *MedeA* GUI.

[MPDS](#) [2], is curated and maintained by Pierre Villars, Evgeny Blokhin, and a leading team of experts in materials science and software engineering.

[1] <http://www.mpds.io>

[2] <http://www.materialsdesign.com/datasheet-mpds>

2 The Novel Materials Discovery (NOMAD) Repository

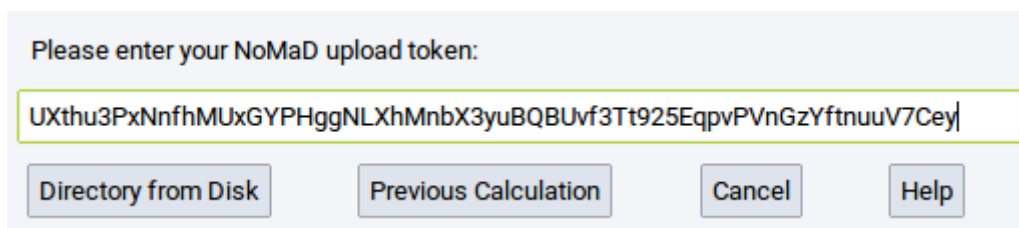
The [NoMaD repository](#) [3] is a free and unrestricted service for publishing and storing the results of materials simulations. To use the service you must sign up for a NoMaD account using their website. The supported file formats and types that can be uploaded are summarized on the NoMaD page [How to upload input and output files](#) [4]. Once signed up your NoMaD account page contains a token which is a text string of 64 alpha-numeric characters. This token, associates file uploads with your NoMaD account.

Within *MedeA* you can either select input and output files in a directory from disk or a previously completed job. During the upload process you will be presented with a progress dialog and, once the upload has completed, a message from the NoMaD servers. The NoMaD parsers inspect every file in the upload to locate any output files produced by any of the supported calculation codes and formats, respectively. If support file formats are detected, these output files are added to the NoMaD repository. Any output files which are not supported by NoMaD are omitted and not added to the repository.

2.1 Define your NoMaD upload token

The NoMaD upload token can be either set in the *MedeA* Preferences (accessible via **File** >> **Preferences** in the main window) or via the *MedeA Upload to NoMaD* dialog. Copy your token from your NoMaD account page and paste it into the relevant field. Then select whether files should be uploaded from a **Directory from Disk** of your computer or from a **Previous Calculation** stored on a *MedeA* JobServer.

Hint: For the *MedeA* JobServer is important to select the proper JobServer via **Job Control** >> **Select Server** >> ...

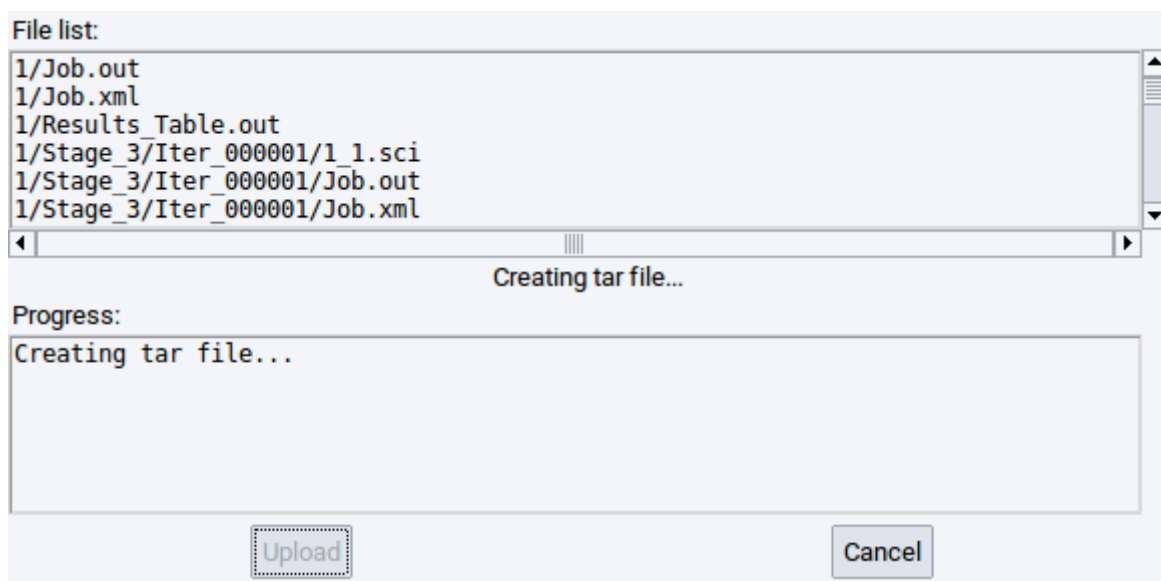
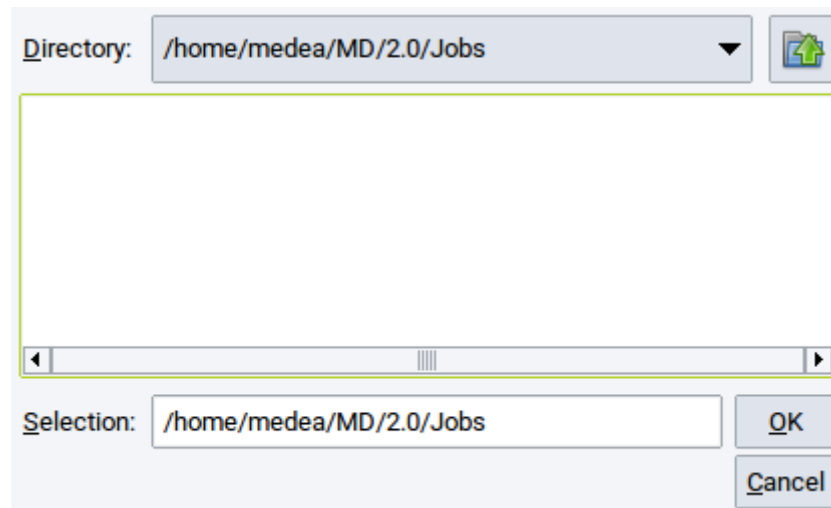


2.2 Upload files from disk

Upon selecting the option **Directory from Disk** a folder browser pops up to navigate to the relevant directory and to select files that should be uploaded. Start the actual upload with the **Upload** option.

[3] <http://repository.nomad-coe.eu/>

[4] <http://www.nomad-coe.eu/the-project/nomad-repository/nomad-repository-howtoupload>



2.3 Upload files from previous jobs

Selecting the option **Previous Calculation** brings up a dialog to select files of relevant jobs. Files are selected if marked with a checkmark. Confirm the selection with **Open**.

Filtering options ↑

User: is anyone ▾

Job name: is anything ▾

Submitted: any time ▾

Started: any time ▾

Finished: any time ▾

Status: is anything ▾

Job Numbers: <= ▾

Hide intermediate files

Number of jobs to display: Refresh

Expand All Collapse All Collapse unselected

Job/File	File size	User
▷ 1394 (5 files) -- PAGs add relevant QSPR descriptors to revised structure list		
▷ 1393 (5 files) -- PAGs add relevant QSPR descriptors to revised structure list		
▷ 1390 (78 files) -- PAGs revised structure list		
▷ 1383 (5 files) -- PEGs add descriptors to revised structure list		
▷ 1382 (42 files) -- PEGs revised structure list		
▷ 1381 (5 files) -- PPGs add descriptors to revised structure list		
▷ 1380 (37 files) -- PPGs revised structure list		
▽ 1377 (19 files) -- (Li I)4 (Fm-3m) ~ Lithium iodide - alpha (ICSD #414244)_1 SP (VASP)		
CONTCAR	523 B	
EIGENVAL	4.1 kB	
IBZKPT	657 B	
INCAR	590 B	
Job.out	3.8 kB	
Job.xml	1.5 kB	
KPOINTS	46 B	
OSZICAR.out	1.2 kB	
OUTCAR.out	52.1 kB	
POSCAR	310 B	
POTCAR	353.0 kB	
PROCAR	18.6 kB	
VASP.out	1.0 kB	

3991 files in 50 jobs over 542 matching jobs 1 selected files (1.3 kB) More

Open Cancel

2.4 Monitor file upload

Once the upload was successfully started the progress is monitored. The upload is complete once the message `Upload finished` appears in the dialog. To continue working with the *MedeA* GUI click on `Close`.

File list:

1377/initial.sci

Upload finished.

Progress:

% Total	% Received	% Xferd	Average Speed	Time	Time	Time	Current
			Dload	Upload	Total	Spent	Left
							Speed
1 10588	100	114	0	0	1527	0	1540

Upload Close