

MedeA Databases

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MedeA uses a variety of databases. Some are structure databases such as [COD](#), [NCD](#), [ICSD](#), and [Pearson](#), materials phase diagrams such as [MSI Phase Diagrams](#), and others that contain user-generated results (MaterialsDesign.db) and internal data (MedeA.db) like potentials and parameters used in *VASP* calculations. For more information see the InfoMaticA section. *MedeA 3.8* uses SQLite as the default database management system. However, the Microsoft SQ server *MSQL* (Windows) and the *MySQL* database server (Linux) of previous *MedeA* versions are still supported.

All the database files (.db) are located by default in the installation directory *MD/Databases*. The primary databases that *MedeA* uses to run calculations are *MDJobs.db* and *MedeA.db*. You can read the contents of these databases using the `sqlite3` [1] program.

If necessary you can change the location of the SQLite database files and also their paths in the *MedeA* database settings (**File** >> **Databases**).

In case of missing databases or if they are corrupted you can download zipped database file (.dbz) from the Materials Design server update.materialsdesign.com/db [2]. To access the database files on the Materials Design server please use the credentials of your Materials Design account, i.e. the same username and password to access my.materialsdesign.com [3]. Please make sure the downloaded file has an extension *.dbz (except for the MSI Pphase Diagram file being `msipd.db`).

Once downloaded, please save .dbz file(s) or `msipd.db` to the directory *MD/Databases* and restart the *MedeA GUI*. Upon restarting the *MedeA GUI*, a window appears to raise the fact that a new database file was found. If you confirm with **OK** the database is automatically extracted and installed. You only need these database files on the computer that has the *MedeA GUI* installed. You do not need these database files on computers that serve only as JobServer and TaskServer. If you need to specify or check the database files, click **File** >> **Databases...** and update them if necessary.

After you restarted the *MedeA GUI*, start *InfoMaticA*: **Tools** >> **InfoMaticA** , followed by **InfoMaticA** >> **Search** . With the menu sequence **Options** >> **Databases** in the *InfoMaticA* search dialogue make sure that all available databases are checked with a check-mark.

1 Databases on network shared drives

If the *MD* directory is installed on an NFS files system, *MedeA* may not be able to write to SQLite database files. In this case, it is recommended to place these database files in a user's home directory (where it is sqlite-compatible) and create symbolic links to them in the *MD/Database* on the NSF file system:

```
ln -s /<NFS_drive>/MD/Databases/Jobs.db /home/medea/Databases/Jobs.db
```

[1] <https://sqlite.org/cli.html>

[2] <http://update.materialsdesign.com/db>

[3] <http://my.materialsdesign.com/user>