

# OQMD - Installation instructions

Step by step instructions to install the qmpy package:

- You need to have several packages installed for the pip install to work:

```
sudo apt install mysql-server  
sudo apt-get install libmysqlclient-dev  
sudo apt-get install libmariadbclient-dev  
sudo apt-get install libgraphviz-dev
```

- You also need to set up your MySQL, there are some instructions here:

<https://www.digitalocean.com/community/tutorials/how-to-install-mysql-on-ubuntu-18-04>

You've already installed MySQL, so you just have to execute Steps 2 and 3. When creating the user, it's best to use the same as your login for your work station.

- Then it's best to setup a new conda environment

```
conda create -yn qmpy python=3  
conda activate qmpy
```

- Next, install `qmpy` in your new environment:

```
pip install qmpy
```

If you don't want to install the HUGE database in the "/var/lib/mysql" default directory (it saturated the memory in my "/" directory where the operating system is), follow these instructions

<https://www.digitalocean.com/community/tutorials/how-to-move-a-mysql-data-directory-to-a-new-location-on-ubuntu-16-04> to point mysql to another direction.

- Now we follow the instructions on [how to set up the database](#) from the OQMD website. However, the final command:

```
mysql < qmdb.sql
```

Needs to be executed with the password option (`-p`) enabled (not sure how to save this password somewhere). Moreover, you first have to set up a database in MySQL to actually be able to execute this command. Start up MySQL:

```
mysql -p
```

Then execute the following:

```
CREATE DATABASE qmdb_prod;
```

This should return: Query OK, 1 row affected (0.00 sec)

Leave MySQL with `exit`, and then also supply this database to the MySQL command to load the OQMD data:

```
mysql -p -D qmdb_prod < qmdb.sql
```

This command will take some time, so make sure to run it in a `screen` if you have internet connection issues.

- Now comes the fun part (I know what you're thinking: even more fun?! 🤖): You have to change the DATABASE settings in `qmpy/db/settings.py`. Now, for the average user, this is completely not clear. Especially since you have to go into the code and hardcode the changes (I'm not sure when these environment variables defined here are loaded, but sure as hell not when you start their IPython terminal). Anyways, my ranting aside, you can find the file you need to adjust here:

```
vim $CONDA_PREFIX/lib/python3.9/site-packages/qmpy/db/settings.py
```

There will be a DATABASE variable defined here, looking like this:

```
DATABASES = {
    "default": {
        "ENGINE": "django.db.backends.mysql",
        "NAME": os.environ.get("qmdb_v1_1_name"),
        "USER": os.environ.get("qmdb_v1_1_user"),
        "PASSWORD": os.environ.get("qmdb_v1_1_pswd"),
        "HOST": os.environ.get("qmdb_v1_1_host"),
        "PORT": os.environ.get("qmdb_v1_1_port"),
    }
}
```

You will have to change it to something like this:

```
DATABASES = {
    "default": {
        "ENGINE": "django.db.backends.mysql",
        "NAME": 'qmdb_prod', # os.environ.get("qmdb_v1_1_name"),
        "USER": os.environ.get("qmdb_v1_1_user"),
        "PASSWORD": <YOUR_PASSWORD>, # os.environ.get("qmdb_v1_1_pswd"),
        "HOST": 'localhost', # os.environ.get("qmdb_v1_1_host"),
        "PORT": os.environ.get("qmdb_v1_1_port"),
    }
}
```

This is assuming you have used `qmdb\_prod` for your database name. Don't forget to change the password which you set up for your user, i.e. the user with your username on your workstation.