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qmpy Documentation May 23, 2014 0.4.9 Scott Kirklin   Release

document

index::doc

qmpy is the backend responsible for creating and running the Open Quantum Materials Database (http://oqmd.orghttp://oqmd.org). The OQMD is a project created in Chris Wolverton's group at Northwestern University (http://wolverton.northwestern.eduhttp://wolverton.northwestern.edu).

Installation $getting_started : installationgetting_started : qmpygetting_started :: doc$

From repo $getting_started : from - repoInstallqmpywithpiporeasyinstall :$

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or:

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noticenoteNote: Using pip or easy_install to install scipy or numpy can be unreliable. It is better to install from a proper repository for your linux distribution. However, if that version of SciPy is earlier than 0.12.0 you will need to obtain another installation. If necessary, you can obtain the needed libraries with:

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From GitHub repo $getting_started : from - github - repoObtainthesourcewith :$

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Be aware that f you want to install qmpy from source, you will be responsible for ensuring that you have all of the following required packages installed.

Required Packages $getting_started : required - packagesitemize$

Django (https://www.djangoproject.com/https://www.djangoproject.com/)

Numpy (http://www.numpy.org/http://www.numpy.org/)

Scipy (http://www.scipy.org/http://www.scipy.org/)

PyYAML (http://pyyaml.org/http://pyyaml.org/)

python-MySQL (https://pypi.python.org/pypi/MySQL-pythonhttps://pypi.python.org/pypi/MySQL-python)█

python-memcached

django-extensions

PuLP (https://pythonhosted.org/PuLP/https://pythonhosted.org/PuLP/) (required for grand canonical linear programming and high-dimensional phase diagram slices)