Open source PyMOL 2.4 for Windows

This repository provides a method to install PyMOL v2.4 by Anaconda on Windows.

Download & Instalação

Follow these steps to install PyMOL v2.4:

1. Install Anaconda

Download Anaconda and install it.

2. Create a environment on Anaconda

Open `Anaconda Prompt`, you can open it by typing`Anaconda Prompt` in the search bar, located in the bottom left corner. With the `Anaconda Prompt` open, run:

```
conda create -n pymol python=3.7
```

Then, activate the `pymol` environment:

```
conda activate pymol
```

3. Install required Python packages

Still on `Anaconda Prompt`, run:

- pip 3:

```
conda install -c anaconda pip
```

- Numpy:

```
pip install numpy
```

- PMW:

```
pip install pmw
```

- pyqt5:

```
pip install pyqt5
```

4. Download PyMOL whl files

Download pre-compiled Open-Source PyMOL wheel files, compatible with Python 3.7.x and Windows 64-bit, from the links below:

- pymol-launcher
- pymol

Note: You can check Python version on anaconda by typing `python --version`.

If you are using a different Python version or Windows 32-bits, please there are other pre-compiled versions here.

The filename structure is the following:

```
1   pymol-2.4.0a0-cp37-cp37m-win_amd64.whl
2            \         \          \
3             \         \          \__ for 64 bit Windows
4              \         \
5               \          _____ for Python 3.7.x
6                \
7                 _____ PyMOL version 2.4.0a0
```

5. Install wheel files

In the `pymol` environment on Anaconda, switch to download directory (`C:\Users\username\Downloads`):

```
cd Downloads
```

Then, install `pymol_launcher-2.1-cp37-cp37m-win_amd64.whl` by typing:

```
pip install --no-index --find-links="%CD%" pymol_launcher-2.1-cp37-cp37m-win_amd64.whl
```

Finally, to install `pymol-2.4.0-cp37-cp37m-win_amd64.whl`, run:

```
pip install --upgrade --no-deps pymol-2.4.0-cp37-cp37m-win_amd64.whl
```

Note: If you downloaded different files in **Step 4**, replace `pymol_launcher-2.1-cp37-cp37m-win_amd64.whl` and `pymol-2.4.0-cp37-cp37m-win_amd64.whl` by the downloaded wheel files.

6. Launch PyMOL v2.4

In the activate `pymol` environment on Anaconda, run:

```
pymol
```

Then, PyMOL v2.4 will be launched and ready to go.