

Alternative methods for installing Quantum ESPRESSO

Linux

1. Install Quantum ESPRESSO via the command "sudo apt-get install quantum-espresso"

Windows 10

1. If you don't have the Fall Update to Windows 10, turn on developer mode (Settings > Update & Security > For Developers and select "Developer mode")
2. Enable the Windows Subsystem for Linux (Control panel > Programs > Turn Windows Feature On or Off > Tick "Windows Subsystem for Linux")
3. Reboot
4. Install "Ubuntu" from the Microsoft Store (Microsoft Store > search for "ubuntu" or go to <https://www.microsoft.com/store/productId/9NBLGGH4MSV6> > click "Get" > "Install")
5. Launch the app "Ubuntu"
6. Create a username and password
7. Install Quantum ESPRESSO by entering the commands "sudo apt-get update" and then "sudo apt-get install quantum-espresso"

Note that if you want to access files on your Windows machine from within the Ubuntu shell they can be found at "/mnt/c/"

MacOS

1. Install brew (in the terminal enter the command '/bin/bash -c "\$(curl -fsSL <https://raw.githubusercontent.com/Homebrew/install/HEAD/install.sh>)"')
2. Install various requisite packages ("brew install wget gcc gfortran fftw lapack openblas open-mpi eigen")
3. Download Quantum ESPRESSO ("wget -c <https://github.com/QEF/qe/releases/download/qe-6.6/qe-6.6-ReleasePack.tgz>" and then "tar xfvz qe-6.6-ReleasePack.tgz")
4. Move into the directory "qe-6.6" and run the command './configure CPP="gcc -E"'
5. In the file "make.inc"..
 1. at line 36 delete the hash at the beginning of the line
 2. at line 48 change "D__FFTW3" to D__FFTW
 3. at line 154 remove everything after the equals sign so it simply reads "FFTLIB = "
6. Compile Quantum ESPRESSO (enter the command "make pw pp")
7. Add Quantum ESPRESSO to your path (export PATH=\$PATH:/path/to/qe-6.6/bin)