

## Quantum Espresso – Download and Compilation Instructions

For WINDOWS (i.e. Ubuntu via WSL):

1. Download QE V.7.2 from: <https://www.quantum-espresso.org/download-page/>
  - a. NOTE: You will be asked to register an account. This is free and should require minimal setup.
2. Copy the downloaded “qe-7.2-ReleasePack.tar.gz” file to your SOFTWARE directory (or wherever you would like to install)
3. Untar with the following: `tar -xvzf qe-7.2-ReleasePack.tar.gz`
4. Change to the qe-7.2 directory (i.e. `cd qe-7.2`)
5. Perform the following commands:
  - a. `sudo apt-get update`
  - b. `sudo apt-get upgrade`
  - c. `sudo apt install git`
  - d. `sudo apt install gcc`
  - e. `sudo apt install gfortran`
  - f. `sudo apt install libfftw3-dev`
  - g. `sudo apt install make`
6. Now we should be set to compile the software with the following:
  - a. `./configure`
  - b. `make all`

For MacOS:

1. Download QE V.7.2 from: <https://www.quantum-espresso.org/download-page/>
  - a. NOTE: You will be asked to register an account. This is free and should require minimal setup.
2. Copy the downloaded “qe-7.2-ReleasePack.tar.gz” file to your SOFTWARE directory (or wherever you would like to install)
3. Untar with the following: `tar -xvzf qe-7.2-ReleasePack.tar.gz`
4. Change to the qe-7.2 directory (i.e. `cd qe-7.2`)
5. Try compiling. Your system already has the appropriate libraries.
  - a. `./configure`
  - b. `make all`
6. If this resulted in any errors, fret not! We will troubleshoot together!