Quantum ESPRESSO for Windows Installation Manual

October 7, 2020

1. Installation of Quantum ESPRESSO

    i.   Download the QE installer from the following links.

    64 bit OS, parallel computing with MPICH (usually selected here)

https://winmostar.com/wm/cygwin_wm/packages/qe-5.2.1-64bit-mpich2.exe

    64 bit OS, serial computing with MPICH

https://winmostar.com/wm/cygwin_wm/packages/qe-5.2.1-64bit-serial.exe
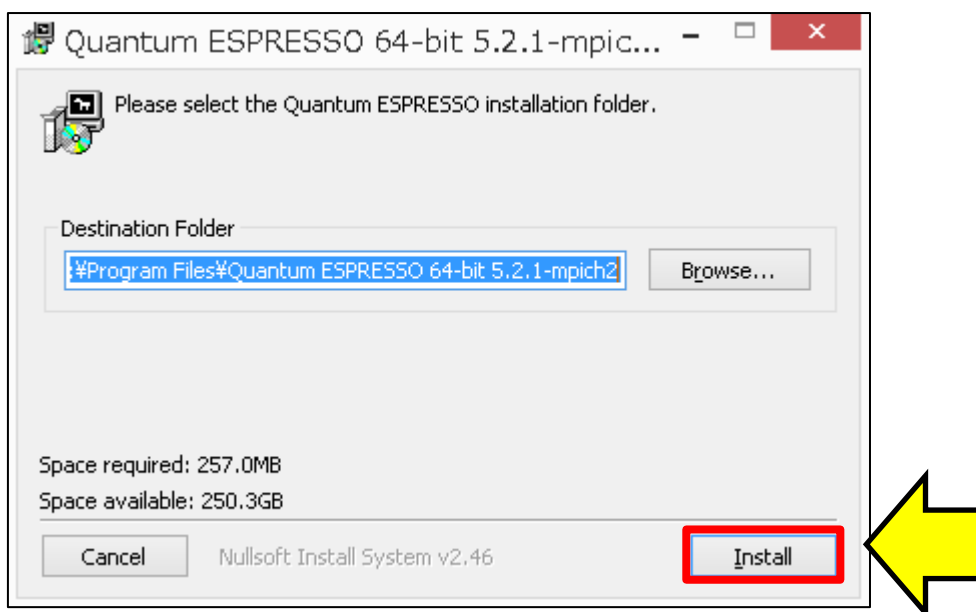
    32 bit OS, parallel computing with MPICH

https://winmostar.com/wm/cygwin_wm/packages/qe-5.2.1-32bit-mpich2.exe

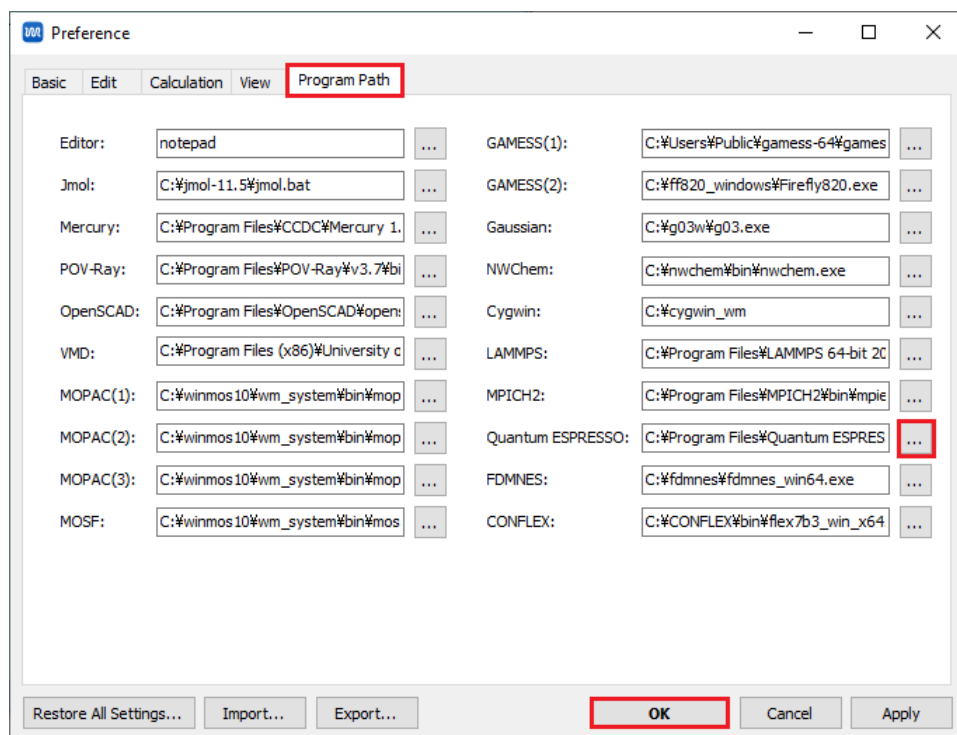   32 bit OS, serial computing with MPICH

https://winmostar.com/wm/cygwin_wm/packages/qe-5.2.1-32bit-serial.exe

    ※ Each installer was generated by Axel Kohlmeyer of Temple University.

    ii.   Double-click on the downloaded exe file and press "Install".

    iii.   To set up the path for Winmostar to call Quantum ESPRESSO, click on Tools > Preferences to open the Preference panel of Winmostar. Open the [Program Path] tab of the Preference Panel, click the [...] button of [Quantum ESPRESSO]. Register the pw.exe file in the bin folder of the Quantum ESPRESSO installation folder, and click [OK].

※ By default,"C:¥Program Files¥Quantum ESPRESSO 64-bit 5.2.1-mpich2¥bin¥
pw.exe" When using the 32-bit version, change it to "C:¥Program Files¥ Quantum
ESPRESSO 32-bit 5.2.1-mpich2¥bin¥pw.exe" or your environment.

2. Installation of cygwin_wm

Download the cygwin_wm installer and set up according to the contents of the link below.

(Not necessary if cygwin_wm has already been set up.)

https://winmostar.com/en/gmx4wm_en.html

3. Installation of MPICH

i. Download [mpich2-1.4.1p1-win-ia32.msi] or [mpich2-1.4.1p1-win-x86-64.msi]. If the extension of the downloaded file is changed, set it back to ".msi". If the installed Quantum ESPRESSO version is 32-bit, select 32-bit MPICH, and if it is 64-bit, select 64-bit.

ii. Double-click on the saved msi file and follow the instructions.
(If the installation fails, download and install ".NET Framework 3.5" from https://www.microsoft.com/en-US/download/details.aspx?id=21. .NET Framework 4.5 is installed by default on Windows 8.1/10", but you need to install 3.5 separately)

iii. Start a command prompt from the Start menu with administrative privileges.

iv. Go to the directory where you installed MPICH.
c:¥> cd "c:¥Program Files¥MPICH2¥bin"

v. Execute the following commands.
bin> smpd.exe –install

vi. Click [Tools] → [Preferences] in Winmostar to open the Preference panel. Open the [Program Path] tab of the Panel, and click [...] button of [MPICH2] to register the mpiexec.exe file in the bin folder of the MPICH installation folder. Register the file, and click [OK].

4. Installation of pseudopotentials

i. Right-click on the Winmostar (shortcut or body) icon and click "Run as administrator".
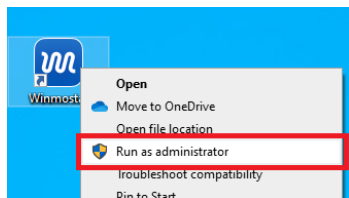

ii. Click [Solid]-[Quantum ESPRESSO]-[Configure].
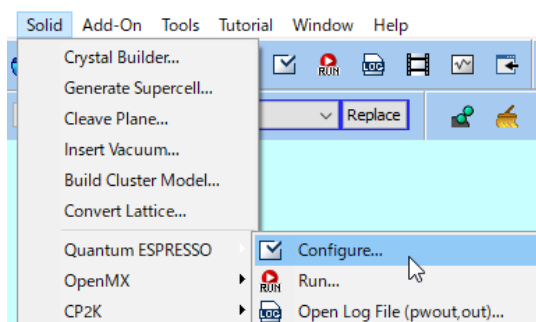
iii. The warning of "Do you want to calculate CH4 by adding hydrogen atom?" is displayed, click the [Yes] button.

iv. When the [Create Cell] dialog box appears, click [OK] with the default value.
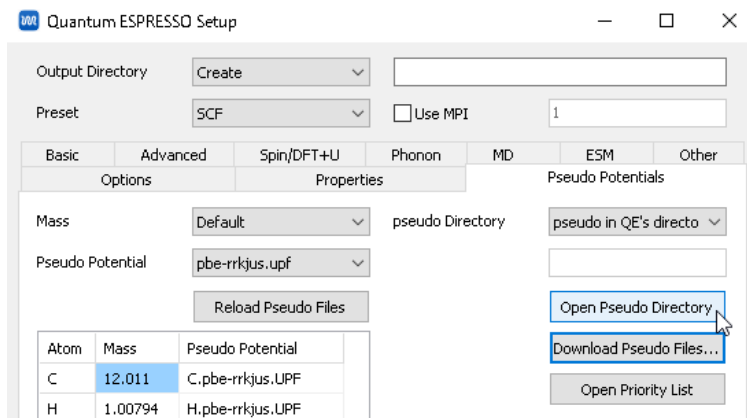
v. Click the [Pseudo Potentials] tab.
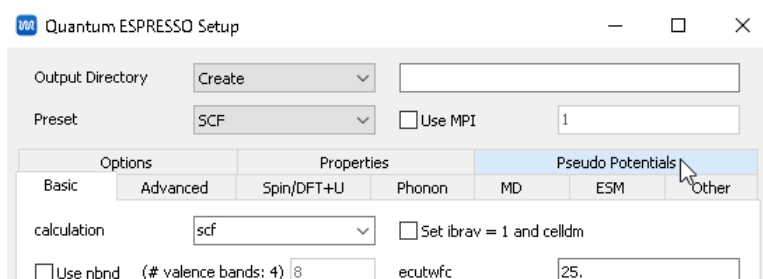
vi. If you do not have internet access, proceed to Step ix.

vii. Click the [Download Pseudo Files] button.
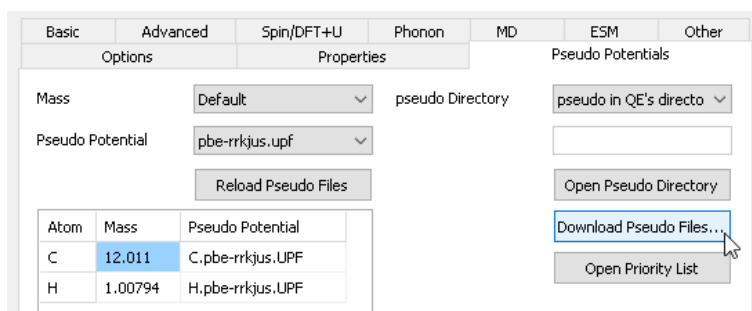
viii. Click the [Start] button in the [Download Files] window. When the process is complete, click the [Close] button.
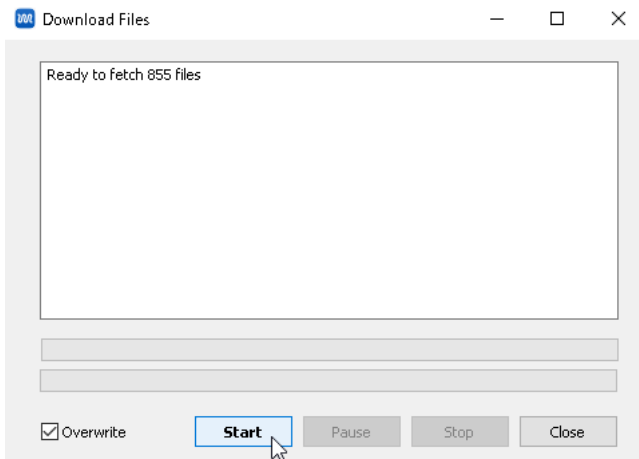
ix.   Manually install pseudo-potential files if necessary. First, click the [Open Pseudo Directory] button and open the pseudo folder in Explorer.

x.   Go to the Pseudopotentials page on the Quantum ESPRESSO official web site. If you want to use something other than PSlibrary which is recommended by default, go to the Original QE PP table on the left side of the page.

xi.   If you want to use PSlibrary, click the element you want to calculate from the periodic table in the above page. Then, right-click the Pseudopotential File with the extension UPF, as shown below, and save the file. The Pseudopotential type and Functional type should be selected so that they are the same for all the elements in the material to be calculated.
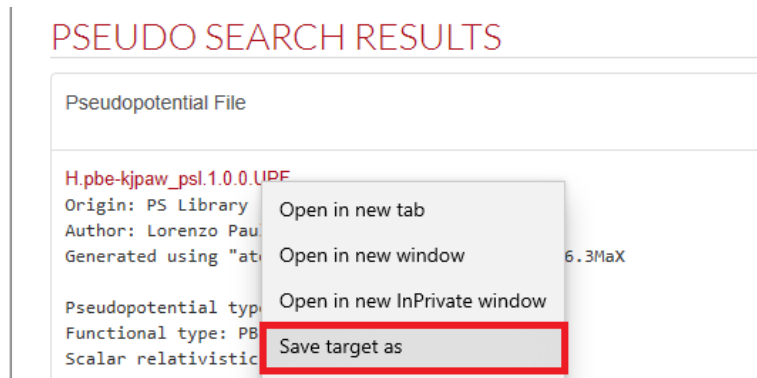

xii.   Copy the saved UPF file to the pseudo folder opened in the previous step ix.

5. Simple operation check

i. Click [File]-[New] in the main menu of Winmostar, then click [Replace] button at the upper center of the main window to create a methane molecule.
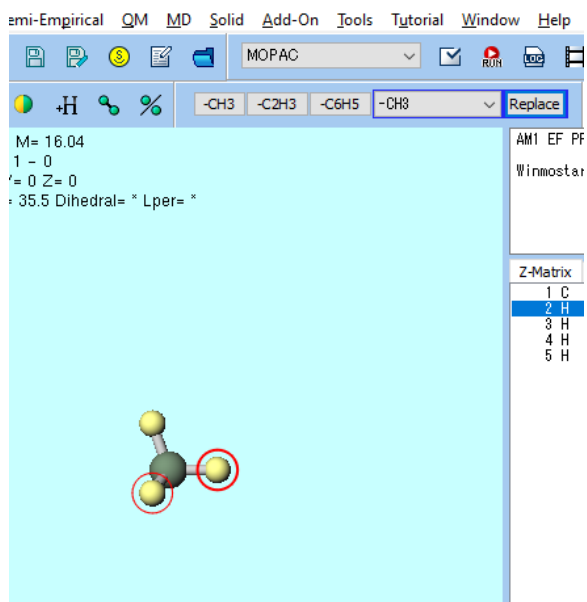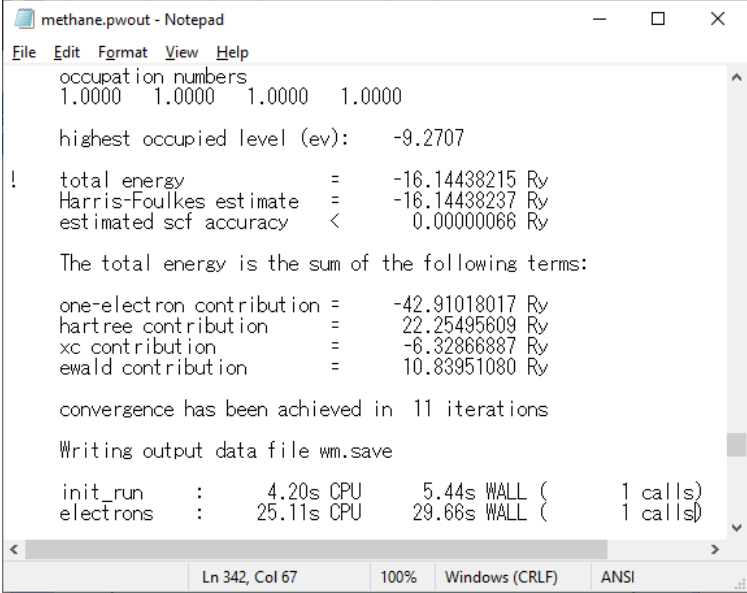
ii. Click [Solid] - [Quantum ESPRESSO] - [Configure].

iii. A dialog box titled "Create Cell" will appear, and press [OK] with the default distance value.

iv. Click [Run] button.
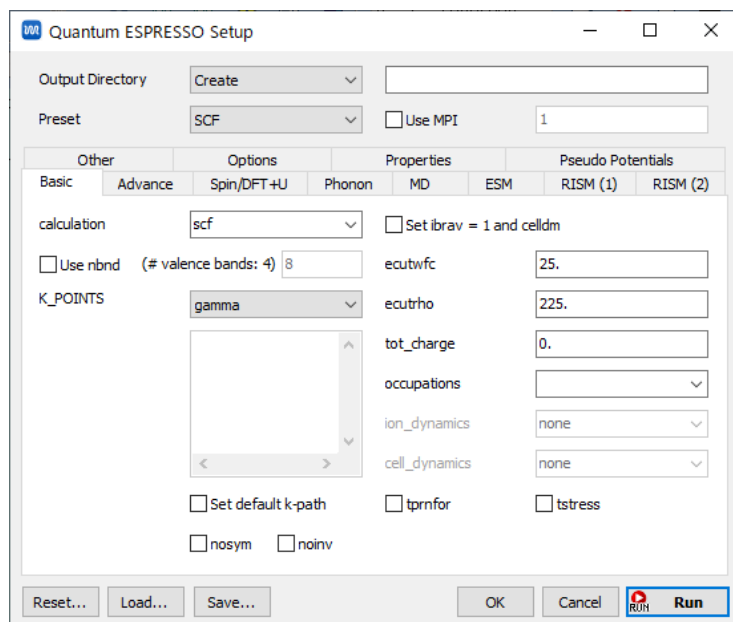
v. A save dialog opens, and when you save it with a suitable name, a black terminal window opens and a lot of messages flows. After a while, the process is over and the terminal window closes.

vi. Click [Solid] - [Quantum ESPRESSO] - [Open Log File], and open the file selected by default

in the dialog. When the calculation succeeded, you will see "convergence has been achieved in ..." at the end of the opened text file.

```
methane.pwout - Notepad                              —    □    ×
File  Edit  Format  View  Help
  occupation numbers
  1.0000   1.0000   1.0000   1.0000

  highest occupied level (ev):    -9.2707

! total energy            =    -16.14438215 Ry
  Harris-Foulkes estimate =    -16.14438237 Ry
  estimated scf accuracy  <      0.00000066 Ry

  The total energy is the sum of the following terms:

  one-electron contribution =    -42.91018017 Ry
  hartree contribution      =     22.25495609 Ry
  xc contribution           =     -6.32866887 Ry
  ewald contribution        =     10.83951080 Ry

  convergence has been achieved in  11 iterations

  Writing output data file wm.save

  init_run    :     4.20s CPU     5.44s WALL (     1 calls)
  electrons   :    25.11s CPU    29.66s WALL (     1 calls)

              Ln 342, Col 67      100%    Windows (CRLF)    ANSI
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