

# Quantum-Espresso 설치 방법 정리

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## 다운로드 및 설치

## 설치파일 Download

<https://www.quantum-espresso.org/login/>

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SOFTWARE	DOCUMENTATION	OTHER
Full source code of QUANTUM ESPRESSO v7.3.1. Ready for compilation in all supported platforms. For more details and instructions see the release notes contained in the archive.	The full documentation bundle of QUANTUM ESPRESSO v7.3.1. Here you can find all the information on the features and capabilities of QUANTUM ESPRESSO.	This archive contains the XSD schemas used by QUANTUM ESPRESSO applications in version 7.3.1 To download the package, press the button below.

[Quantum ESPRESSO V.7.3.1 Doc](#)
[Quantum ESPRESSO V.7.3.1 Schemas](#)

Quantum ESPRESSO V.7.3.1

<https://www.quantum-espresso.org>
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## 압축 풀기

```
(base) lsp32@celinux2:~$ tar -zxvf qe-7.3.1-ReleasePack.tar.gz |
```

## configure 진행 (prefix 소용 없는것으로 확인)

```
(base) lsp32@celinux2:/usr/local/bin$ ./configure --prefix=/usr/local/bin
```

```
The following libraries have been found:
BLAS_LIBS= -lblas
LAPACK_LIBS=-L/usr/local/lib -llapack -lblas
FFT_LIBS= -lfftw3
```

## 컴파일 진행

```
(base) lsp32@celinux2:~/qe-7.3.1$ make all
```

make 빌드 규칙 중 all참고

```
all : pwall cp ld1 tddfpt hp xspectra gwl kcw
```

```
mpif90 -g -o bse_main.x \
    bse_main.o libbse.a ../../PW/src/libpw.a ../../KS_Solvers/libks_solvers.a ../../
dhkdwk/qe-7.3.1/Modules/libqemod.a /home/dydtkddhkdwk/qe-7.3.1/upflib/libupf.a /home/
ib.a /home/dydtkddhkdwk/qe-7.3.1/FFTXlib/src/libqefft.a /home/dydtkddhkdwk/qe-7.3.1/L
k/qe-7.3.1/UtilXlib/libutil.a /home/dydtkddhkdwk/qe-7.3.1/MBD/libmbd.a -L/home/dydtk
b/src -ldevXlib -L/usr/local/lib -llapack -lblas -lfftw3 -lblas ../../pw4gww/f
./pw4gww/mp_wave_parallel.o ../gww/libgww.a ../minpack/minpacklib.a
( cd ../../bin ; ln -fs ../GWW/bse/bse_main.x . )
make[2]: Leaving directory '/home/dydtkddhkdwk/qe-7.3.1/GWW/bse'
make[1]: Leaving directory '/home/dydtkddhkdwk/qe-7.3.1/GWW'
(base) lsp32@celinux2:~/qe-7.3.1$
```

## 설치

## 빌드 완료 확인

```
(base) lsp32@celinux2:~/qe-7.3.1$ cd bin/
(base) lsp32@celinux2:~/qe-7.3.1/bin$ ls
alpha2f.x      epsilon.x      kcwpp_sh.x      ph.x           pw2bgw.x      spectra_correction.x
average.x      ev.x           kpoints.x        phcg.x         pw2critic.x    sumpdos.x
band_interpolation.x  fermi_proj.x   lambda.x         plan_avg.x     pw2gw.x        turbo_davidson.x
bands.x        fermi_velocity.x  ld1.x           plotband.x     pw2wannier90.x  turbo_eels.x
bse_main.x     fqha.x         manycp.x         plotproj.x     pw4gww.x        turbo_lanczos.x
cell2ibrav.x   fs.x           manypw.x         plotrho.x      pwcond.x        turbo_magnon.x
cp.x           gww.x          matdyn.x         pmw.x          pwi2xsf.x       turbo_spectrum.x
cphp.x         gww_fit.x      molecularnexus.x postahc.x       q2qstar.x       wannier90.x
d3hess.x       head.x         molecularpdos.x postw90.x       q2r.x           wannier_ham.x
dist.x         hp.x          neb.x            pp.x           risml.d.x       wannier_plot.x
dos.x          ibrav2cell.x   open_grid.x      ppacf.x        scan_ibrav.x    wfck2r.x
dvscf_q2r.x    initial_state.x oscdft_et.x      pprism.x       simple.x         wfdd.x
dynmat.x       kcw.x          oscdft_pp.x      projwfc.x     simple_bse.x    xspectra.x
epa.x          kcwpp_interp.x path_interpolation.x pw.x          simple_ip.x
```

## 환경 변수에 프로그램 경로 추가

```
(base) lsp32@celinux2:~/qe-7.3.1/bin$ pwd
/home/dydtkddhkdwk/qe-7.3.1/bin
```

```
135
136
137 export PATH="/home/dydtkddhkdwk/qe-7.3.1/bin:$PATH"
```

```
(base) lsp32@celinux2:~/qe-7.3.1/bin$ source ~/.bashrc
```

```
(base) dydtkddhkdwk@DESKTOP-3IBJ11D:~$ which pw.x
/home/dydtkddhkdwk/qe-7.3.1/bin/pw.x
```

## 참고 자료

참고 영상

<https://www.youtube.com/watch?v=-5fcsJILc6U>