
2023 School on Many-Body Calculations using EPW and BerkeleyGW

Convergence tests of GW calculations using BerkeleyGW

Hands-on session (Fri.3)

Hands-on based on QE-v7.2 and BerkeleyGW-3.0.1

Exercise 3 (convergence)

In this exercise we will go through the process of properly converging a GW calculation for silicon. The mean-field calculation has already been performed using a $2 \times 2 \times 2$ k-grid and a 60 Ryd wavefunction cutoff.

The basic goals are the following:

1. Understand the steps of the convergence process.
2. Estimate the error from using a finite number of bands and G-vectors.

The stretch goals are:

1. Check convergence when using the static remainder.
2. Check convergence with wavefunction cutoff.
3. Check convergence with q-grid.

Setup Instructions

To run this tutorial we will use an interactive session on Frontera. You should already have created your working directory (SCRATCH/EP-SCHOOL.BGW), so you just need to copy and extract the tutorial folder:

```
$ cd $SCRATCH/EP-SCHOOL
$ cp /work2/06868/giustino/SCHOOL/Fri.3.DelBen.tar .
$ tar -xvf Fri.3.DelBen.tar
$ cd convergence
```

To start the interactive session use:

```
$ /work2/06868/giustino/SCHOOL/BGW/bgw_interactive
```

To run the exercise, after you created an interactive session, enter the directory:

```
$ cd $SCRATCH/EP-SCHOOL/convergence/
```

and follow the instructions given in the README.md files.