

## 2023 School on Many-Body Calculations using EPW and BerkeleyGW

### GW calculations of Silicon using BerkeleyGW

#### Hands-on session (Thu.3)

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

### BerkeleyGW Overview

In this tutorial you will use the BerkeleyGW software package to calculate the GW band structure of silicon and subsequently use the GW's results for the GW to calculate the absorption spectrum via Bethe–Salpeter equation (BSE) approach. An overview of the GW-BSE workflow as implemented in BerkeleyGW is given in Fig. 1.

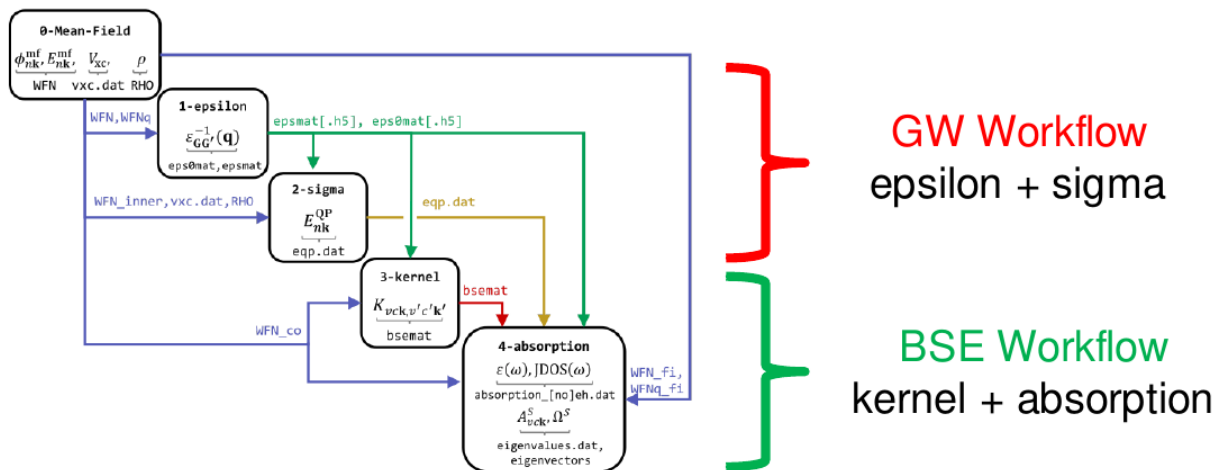


Fig. 1 Shown is the typical workflow, including the required input and output files, for the GW-BSE calculations with BerkeleyGW.

In order to compute GW quasiparticle energies and optical absorption spectra including excitonic effects with BerkeleyGW, one is required to run the following steps:

0. A mean-field program of their choice, such as Quantum ESPRESSO, PARATEC, Abinit, PARSEC, OCTOPUS, JDFTx and SIESTA, and generate a set of files.
1. **epsilon** module computes the polarizability function, its frequency dependence and generate the dielectric matrix and its inverse  $\epsilon^{-1}$ .
2. **sigma** module computes the screen coulomb interaction  $W$  necessary to compute the self-energy  $\Sigma$  and solves the GW Dyson's equation to compute the quasiparticle energies of the system.
3. **kernel** module computes the direct and exchange BSE kernel matrix elements on a coarse k-point grid.
4. **absorption** module interpolates the BSE kernel matrix elements onto a fine k-point grid, diagonalize the BSE Hamiltonian, and compute the optical absorption spectrum.

---

In this tutorial we will use Quantum ESPRESSO to perform the mean-field calculations, generating the various wavefunctions (WFN) and other inputs necessary to run BerkeleyGW. In exercise 1 (gw) we will use the epsilon and sigma modules of BerkeleyGW to evaluate the GW band structure of silicon. In exercise 2 (bse) we will use kernel and absorption modules of BerkeleyGW to evaluate the BSE optical absorption spectrum of silicon.

### Exercise 1 (gw)

In this exercise we will calculate the quasiparticle band structure of silicon using the LDA and GW approximations. We will perform the starting mean-field calculation using Quantum ESPRESSO (QE).

The basic goals are the following:

1. Understand the basic workflow of BerkeleyGW, and the relation between the k-grids, wavefunctions, and the epsilon, sigma, and inteqp codes.
2. Run a basic GW calculation on silicon with the generalized plasmon pole (GPP) model.
3. Construct an interpolated band structure via scissors parameters and Inteqp.

### Setup Instructions

To run this tutorial we will use an interactive session on Frontera. First copy and extract the tutorial folder:

```
$ cd $SCRATCH
$ mkdir EP-SCHOOL ; cd EP-SCHOOL
$ cp /work2/06868/giustino/SCHOOL/tutorials/Thu.3.DelBen.tar .
$ tar -xvf Thu.3.DelBen.tar
$ cd gw
```

To start the interactive session use:

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

Note that in order to run the tutorial you need to be on an interactive session. The interactive session will last for 1 hour. After 1 hour the interactive session will expire and you'll need to create a new one by typing the command above. The script will automatically check if you already have an active interactive session and won't allow to have more than one. To check if you already have an active interactive session use the command:

```
$ squeue -u $USER
```

To cancel an existing interactive session use:

```
$ scancel JOBID
```

providing as JOBID argument the job ID number that appears under JOBID column after running squeue -u \$USER command.

To run the exercise, after you created an interactive session (see previous section), enter the directory:

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

---

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

At the end of the exercise you'll be able to plot the LDA and GW band structures. Figure 2 shows the results for your reference.

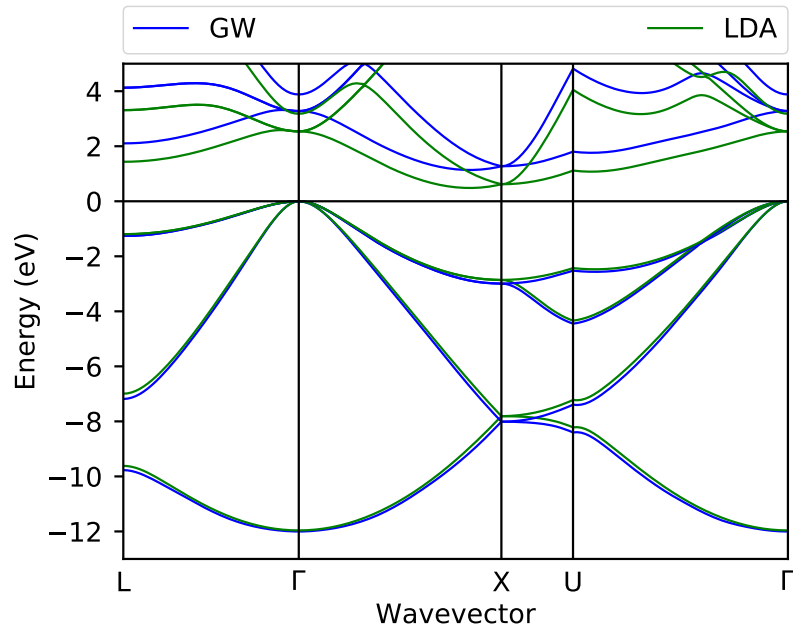


Fig. 2 Shown are the band structures of silicon at the LDA and GW computed by BerkeleyGW in this exercise.