
2023 School on Many-Body Calculations using EPW and BerkeleyGW

Bethe-Salpeter-equation (BSE) calculations of Silicon using BerkeleyGW

Hands-on session (Thu.4)

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

Exercise 2 (bse)

In this exercise we will calculate the optical absorption spectrum of silicon within the GW-BSE formalism. We'll continue from where we left off in the previous exercise where you calculated the quasiparticle band structure of silicon within the GW approximation.

The basic goals are the following:

1. Learn how to use the `kernel` and `absorption` codes.
2. Plot the optical absorption spectrum of silicon with and without electron-hole (e-h) interactions.

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/Thu.4.Li.tar .
$ tar -xvf Thu.4.Li.tar
$ cd bse
```

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.

Note that for running this exercise you would need the results from exercise 1. To facilitate the execution we will reuse your pre-ran solutions from the `1-silicon_gw` from your previous exercise. Check the scripts in the folder to see how the links are created.

At the end of the exercise you'll be able to plot the optical absorption spectra of silicon, BerkeleyGW will provide the spectrum both including and excluding the electron-hole. Figure 1 shows the results for your reference.

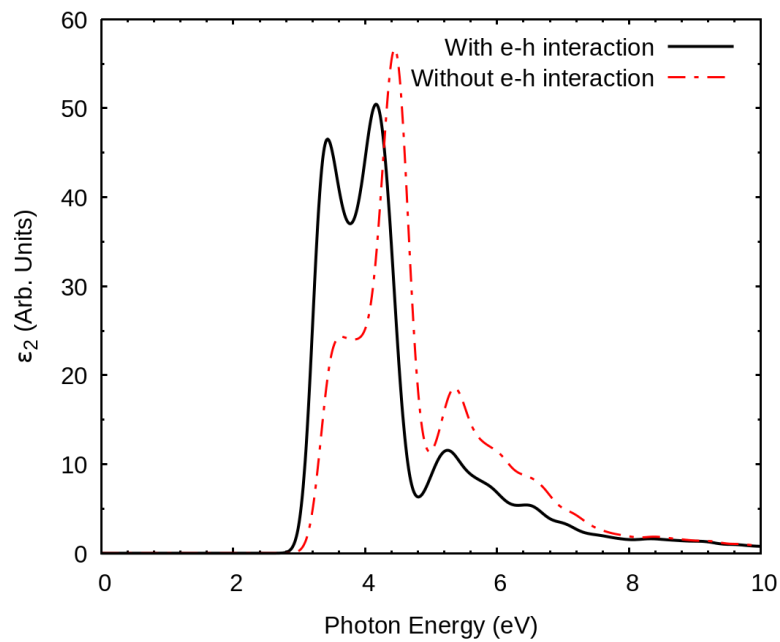


Fig. 1 Shown are the absorption spectra computed by BerkeleyGW including and excluding electron-hole interactions.