2023 School on Many-Body Calculations using EPW and BerkeleyGW

GW and GW-BSE calculations of 2D material using BerkeleyGW: Example of Boron Nitride (BN)

Hands-on session (Fri.4)

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

Exercise 4 (2d material: boron nitride)

In this exercise, we will compute a 2D material, boron nitride (BN). This exercise provides basics of low-dimensional GW calculations using BerkeleyGW, in particular with the Coulomb truncation. We will practice plot exciton wavefunctions and finite-**Q** BSE calculations, which can provide exciton band structures when more **Q**-points are sampled.
The basic goals are the following:

1. Understand the difficulty of **k**-/**q**-meshes convergence in 2D due to the spatial inhomogeneity.
2. Pay attention to the Coulomb truncation scheme that BerkeleyGW adopts for finite systems: 0D, 1D, 2D.

The stretch goals are:

1. Plot the exciton wavefunction .
2. Compute the finite-**Q** BSE.

Setup Instructions

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

```
$ cd $SCRATCH/EP-SCHOOL_BGW
$ cp /work2/06868/giustino/SCHOOL/Fri.4.Li.tar .
$ tar -xvf Fri.4.Li.tar
$ cd 2d-material-bn
```

To start the interactive session use:

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

This practice shows that for low-dimensional materials, Coulomb truncation is an effective approach to speed up the convergence w.r.t. vacuum size. One can plot the exciton wavefunctoins, see Fig. 1 below as an post-processing step. Plotting can be done with either VESTE or XCrysDen. This example also includes a non-zero exciton **Q** point calculation. Exciton band structures can be obtained by including more **Q** points along a path. The finite-**Q** BSE calculations are also an essential step for exciton-phonon coupling calculations, where the electron-phonon matrix elements are also involved.

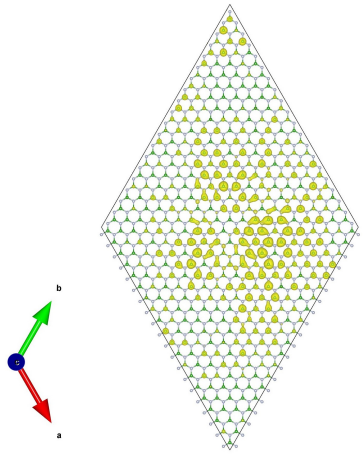

Fig. 1 BN exciton wavefunctions plotted with VESTA.