Hands-On Session 6: Monolayer Boron Nitride

BerkeleyGW Workshop
11/23/2013
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Goals:

1. Demonstrate a GW-BSE calculation for a 2D semiconductor

2. Look at the behavior of $\varepsilon^{-1}_{00}(q)$ for a system with a truncated Coulomb interaction

3. Learn how to use BerkeleyGW's visualization tools to look at the exciton wave function

Instructions:

Please copy the example directory into your scratch directory

>> cp -rP /project/projectdirs/m1694/BGW-2013/6-boron_nitride $SCRATCH/

1-MF

- Please go the directory ``6-boron_nitride/1-mf/``

- Enter each directory in numerical order and follow the instructions in the README files.

Some things to note for 2D calculations:

- The system is in a periodic supercell. Though we will not do so in this calculation, you should always converge the k-grid sampling and amount of vacuum between periodic images.

- The number of nscf bands you will need to generate will increase with the supercell size.

- You do not have to sample k-space in the vacuum direction.

2-BGW

- One you are done with the mean field calculations you can go to the directory ``6-boron_nitride/2-bgw/`` to start the GW calculation

1-Epsilon

- Please follow the instructions in the README file.

- New BGW flag: cell_slab_truncation

Some things to note:

- Coulomb truncation forces $\varepsilon^{-1}_{00}(0)=1$.

- In a 2D system with a truncated Coulomb interaction, it's important to capture the variation in $\varepsilon^{-1}_{00}(q)$ for small q-vectors.

- The location and sharpness of the "dip" in $\varepsilon^{-1}_{00}(q)$ varies with the amount of vacuum.

12x12
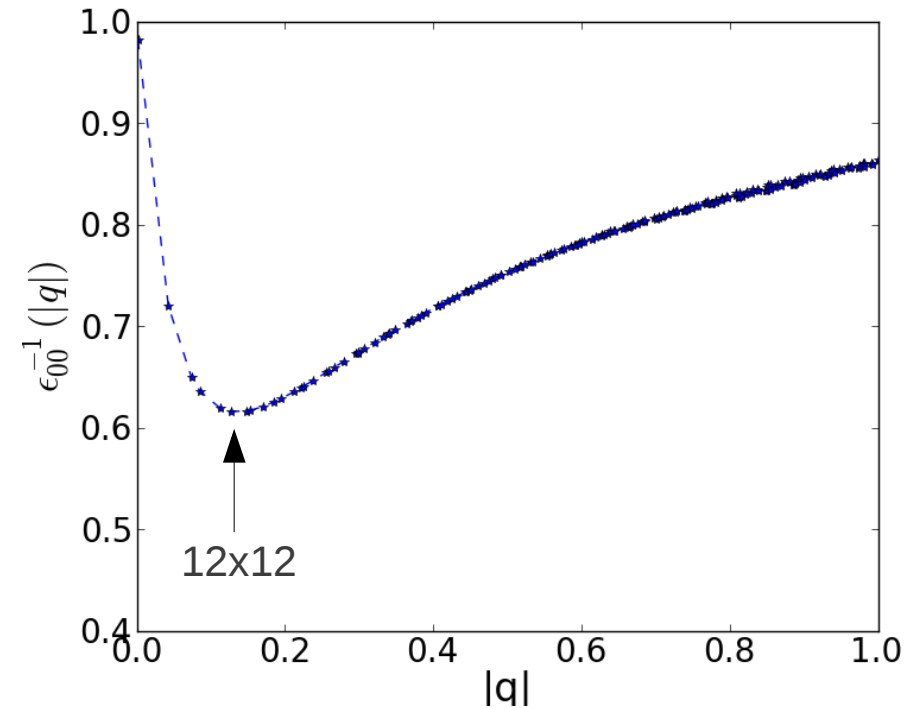
2-Sigma:

- Please follow the instructions in the README file.

Convergence with respect to q-grid sampling used in Epsilon:
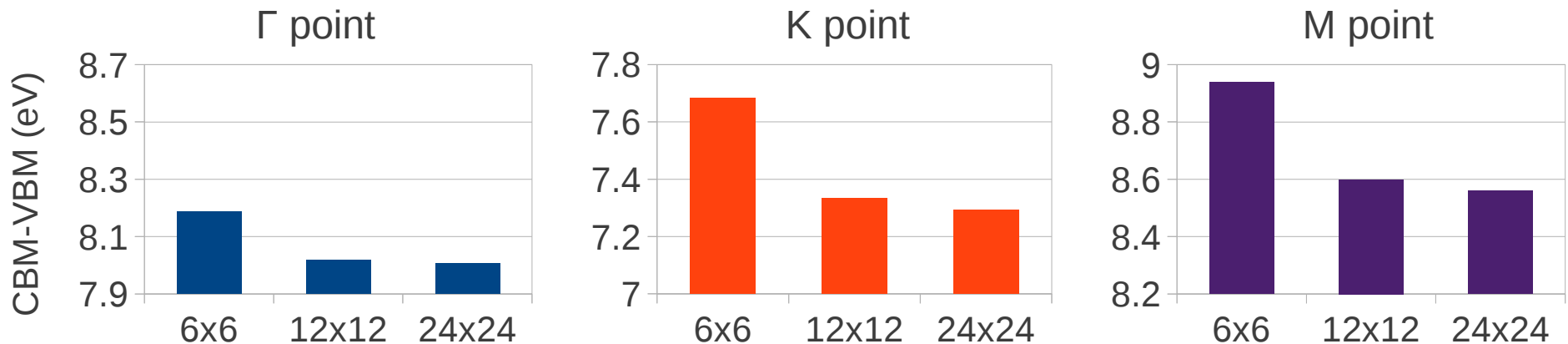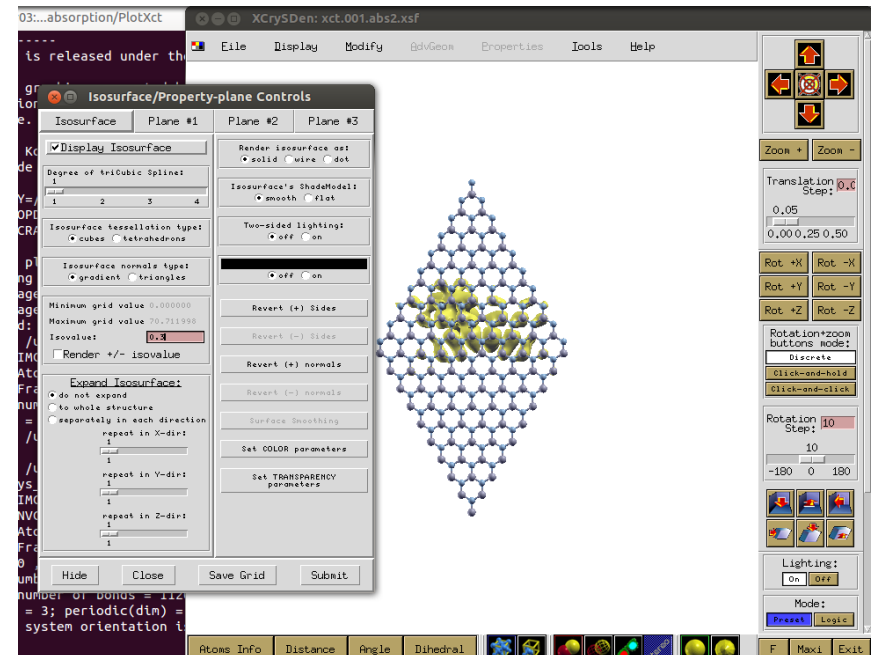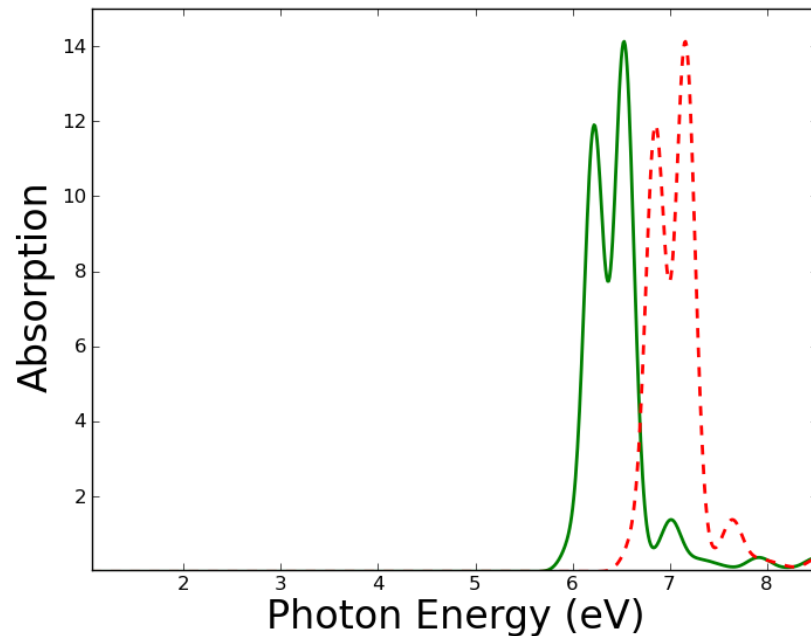

3-Kernel:

- This can be run simultaneously with Sigma.

- Please follow the instructions in the README file.

4-Absorption:

- Please go to the directory 4-absorption and follow the instructions in the README file

PlotXct:

- Please go to the directory 4-absorption/PlotXct and follow the instructions in the README file

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