TUTORIAL 1: BASIC GW CALCULATIONS – SILICON

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1-silicon_GW: Workflow

kgrid.x
wfn_rho_vxc_info.x

BerkeleyGW
1a-silicon_GW: Epsilon: screening as a function of $|q|$
1-silicon_GW: inteqp – interpolated bandstructure

LDA gap: 0.483 eV
GW gap: 1.137 eV
1-silicon_GW: Goals

Basic goals:
1. Understand the basic workflow of BerkeleyGW, and the relation between the \( \mathbf{k} \)-grids, wavefunctions, \( \epsilon \), \( \sigma \), and \( \text{inteqp} \).
2. Run a basic GW calculation on silicon.
3. Construct an interpolated bandstructure using the \text{inteqp} code.

Stretch goals:
1. Compare your Sigma GW results with Hartree-Fock and/or static COHSEX. What inputs are no longer necessary? How do the results compare?
2. Modify the example for GaAs and repeat each step of the calculation.
3. Adapt calculation to use half-shifted \( \mathbf{k} \)-grids.
Logging in with Jupyter

1. Go to [https://jupyter.nersc.gov](https://jupyter.nersc.gov)
2. Log in
3. Click on on the button for "Cori" / "Shared CPU Node"
Logging in with Jupyter

4. Click on "Terminal"
5. Copy the workshop examples to your $SCRATCH folder. Type the following commands into the new Jupyter console:

```bash
# Go to scratch space to run jobs
cd $SCRATCH

# Copy tutorial directory to your directory
cp -rP /project/projectdirs/m3034/vESW_2020/BerkeleyGW/1-silicon_GW .

# Enter your local folder
cd 1-silicon_GW
```
Logging in with Jupyter

6. Navigate to the corresponding tutorial folder

First click here

Then here
7. Once you find the correct folder, right click on the "README.md" file, select "Open With" -> "Markdown Preview"
8. Now, you can work on the terminal, read the instructions (README.md files) and see files all from the same interface.

Hands-on Session: Silicon

Overview

In this session we will calculate the quasiparticle band structure of silicon using the LDA and GW approximations. You will have the option to perform the starting mean-field calculation with a choice of three different DFT codes: PARATEC, Quantum ESPRESSO (QE), or Abinit.

Goals
Final instructions

Always load the berkeleygw/2.1-beta module before running any command!

module load berkeleygw/2.1-beta

Additional resources:
• BerkeleyGW manual: http://manual.berkeleygw.org/2.2/
• 2019 workshop examples: http://workshop.berkeleygw.org