Manual for Calculating Chemical Potentials Using the BoltzWann and CPC Programs

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1 Perform Wannier Calculations Using VASP

1.1 Using VASP to Perform Wannier Calculations

A. `INCAR`: The user must add the tag `LWANNIER90 = .TRUE.` and must also comment out `NPAR = #`; only a single point calculation is needed.

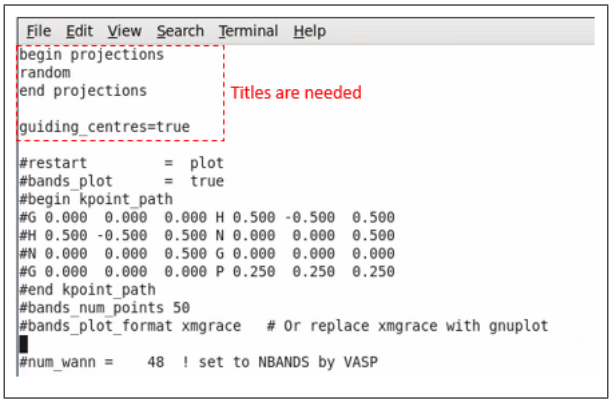
B. `KPOINTS`: Use optimized structure.

C. `POSCAR`: Use optimized structure.

D. `POTCAR`: Use optimized structure.

E. `pbs.sub`: The VASP binary must be compiled with the Wannier code:
```
mpirun -np $NUM_PROCS/home/c9o/hcz/VASP/xt_5.4.1-wannier/oic_opt/vasp_std>stdout
```

F. `wannier90.win`: Add an empty `wannier90.win` file to the directory and add the title commands, as shown below.



Note that `wannier90.win`
is only a seedname and can be renamed if desired.

1.2 Submitting the `pbs` Job

Submit the `pbs` job and the following three files will be produced as ouput:

1. `wannier90.eig`
2. `wannier90.amn`
3. `wannier90.mmn`

Wannier data will automatically write into the empty `wannier90.win` file when done.

1.3 Wannier File Linking

You may need to create a new folder and copy the `wannier90.win` file into it. In addition, copy or link the three generated Wannier output files (`.eig`,`.amn`,`.mmn`) into the same folder. Linking the files may prove more convenient than copying if the files are too large.

```
#PBS -S /bin/bash
#PBS -V
#PBS -N wannier90x
#PBS -m ae
#PBS -M c9o@ornl.gov
#PBS -q cnms10fq
#PBS -l nodes=1:ppn=1
#PBS -l walltime=72:00:00
#PBS -l cput=10000:00:00

echo "-------------------------"
export OMP_NUM_THREADS=1
echo "OMP_NUM_THREADS =" $OMP_NUM_THREADS
echo "-------------------------"
NUM_PROCS=`/bin/awk 'END {print NR}' $PBS_NODEFILE`
echo "Number of processors =" $NUM_PROCS
echo "Node file: $PBS_NODEFILE :"
cat $PBS_NODEFILE
echo "-------------------------"

cd $PBS_O_WORKDIR

echo "Started from `date`"

 /home/c9o/hcz/wannier90-1.2/wannier90.x wannier90
```

only series calculation

pbs linking example; note that the wannier90.x binary can only do series calculations and is not applicable for parallel computing.

1.4 Submitting the pbs Job to the wannier90.x Binary

Submit the pbs to run the wannier90.x binary. When the program is finished, it will create awannier90.chk file. You should now have five files:

1. wannier90.eig
2. wannier90.amn
3. wannier90.mmn
4. wannier90.win
5. wannier90.chk

2 Calculating Thermoelectric Properties via BoltzWann Code

2.1 Revising The `wannier90.win` File to Run BoltzWann Code

A. If you want to calculate thermoelectric properties as a fucntion of chemical potential and temperature, use the following arguments:

```
begin projections
random
end projections

guiding_centres=true

boltzwann = true          • Switch on boltzwann
kmesh = 100               • K meshing, more dense more smooth curve
boltz_mu_min = 7          • Min chemical potential
boltz_mu_max = 9.5        • Max chemical potential
boltz_mu_step = 0.001     • Unit step of chemical potential
boltz_temp_min = 100      • Min temperature
boltz_temp_max = 500      • Max temperature
boltz_temp_step = 100     • Unit step of temperature
boltz_relax_time = 10     • Constant relaxation time, unit in fs
```

B. Alternatively, you may calculate thermoelectric properties as a function of only temperature. In this case you will need to also calculate the density of states (DOS). Use the following arguments:

```
begin projections
random
end projections

guiding_centres=true

boltzwann = true                    • Switch on boltzwann
kmesh = 40                          • K meshing, more dense more smooth curve
boltz_mu_min = 7                    • Min chemical potential
boltz_mu_max = 9.5                  • Max chemical potential
boltz_mu_step = 0.001               • Unit step of chemical potential
boltz_temp_min = 10                 • Min temperature
boltz_temp_max = 300                • Max temperature
boltz_temp_step = 20                • Unit step of temperature
boltz_relax_time = 10               • Constant relaxation time, unit in fs
boltz_calc_also_dos=true            • Switch on DOS calculation
boltz_dos_energy_step = 0.001       • Unit step of DOS
smr_type = gauss                    • Smear type
boltz_dos_adpt_smr = false          • Adopt smear or not
boltz_dos_smr_fixed_en_width = 0.03 • Smear width
```

Note: In order to obtain a smooth relation, reduce the step size.

More details about the BoltzWann commands can be found on page 103 of the BoltzWann manual:

`http://www.wannier.org/doc/user_guide.pdf`

2.2 Preparing a New `pbs.sub` File to Submit a Job

Copy or prepare a new `pbs.sub` file to submit a job. You need to run the `postw90.x` binary to call the BoltzWann program, as shown below.

```
#PBS -S /bin/bash
#PBS -V
#PBS -N electronic
#PBS -m ae
#PBS -M c9o@ornl.gov
#PBS -q cnms10fq
#PBS -l nodes=2:ppn=8
#PBS -l walltime=72:00:00
#PBS -l cput=10000:00:00


echo "-------------------------"
export OMP_NUM_THREADS=1
echo "OMP_NUM_THREADS =" $OMP_NUM_THREADS
echo "-------------------------"
NUM_PROCS=`/bin/awk 'END {print NR}' $PBS_NODEFILE`
echo "Number of processors =" $NUM_PROCS
echo "Node file: $PBS_NODEFILE :"
cat $PBS_NODEFILE
echo "-------------------------"

cd $PBS_O_WORKDIR

echo "Started from `date`"

 mpirun -np $NUM_PROCS /home/c9o/hcz/wannier90-2.0.1/postw90.x wannier90>stdout
```

2.3 Steps After Creating the `wannier90_boltzdos.dat` File

When the job is done, the `wannier90_boltzdos.dat` file will be created. From here, chemical potential can be calculated. The Seebeck coefficient can then be calculated as a function of temperature and chemical potential.

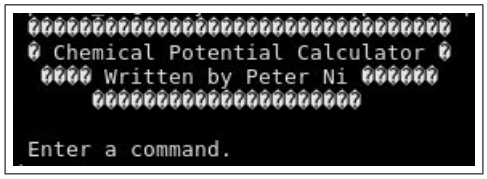
3 Using CPC to Calculate Chemical Potentials

3.1 File Generation and Setup

Generate the `wannier90_boltzdos.dat` file using the instruction sets (1) and (2). Make sure that the `.dat` file is in the `~/cpc/data/` folder, a subfolder in which the program is contained.

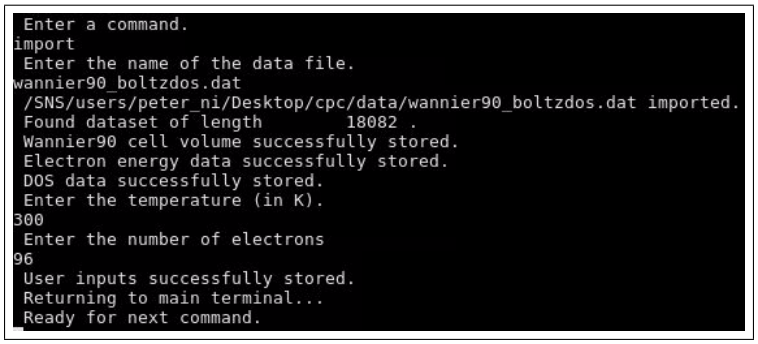
3.2 Running CPC

Find the CPC program `cpclinux.out` in the `~/cpc/` directory and navigate to the folder in the Linux terminal. Launch it in the Linux shell using `./cpclinux.out` and the following prompt will appear:



3.3 Calling the Import Function

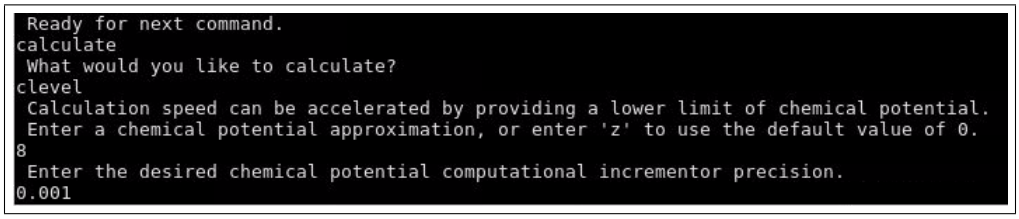
Import the data file by calling `import` in the terminal, and answering the prompts that follow, as shown below:



If a file error is returned, check your spelling and check that the file is in the corrent directory.

3.4 Calling the Calculate Function

To calculate chemical potential (without N- or P-type doping), call the `calculate` function with the `clevel` field, and answer the prompts, as shown below:



Note: A good chemical potential approximation will accelerate computational speed. In addition, using a larger incrementor will also accelerate computational speed, at the expense of precision.

After calling the `calculate` function and answering the prompts, the following output should be printed:

```
Chemical Potential:   8.2540000120643526       eV using a    1.00000005E-03  incrementor and 10^-10
threshold.
<clevel> has been computed.
Took   0.505794942      seconds to compute.
Returning to main terminal...
Ready for next command.
```

3.5 Calling the Calculate Function for N- or P-Type Doping

To calculate chemical potential with N- or P-type doping, once again call the `calculate` function, this time entering either `ndope` or `pdope`, as shown:

```
 Ready for next command.
calculate
 What would you like to calculate?
pdope
 Calculation speed can be accelerated by providing a lower limit of chemical potential.
 Enter a chemical potential approximation, or enter 'z' to use the default value of 0.
8
 Enter the desired chemical potential computational incrementor precision.
0.001
 Enter the carrier concentration in units of (1 * 10^18/cm^3).
1.88
```

Make sure you input the carrier concentration in the correct listed unit, or your chemical potential may be off by many magnitudes.

After running the program, the following output will be displayed:

```
The post p-doped number of electrons is    95.999299649241763

Chemical Potential:   8.1490000070771202       eV using a    1.00000005E-03  incrementor and 10^-10
threshold.
<clevel> has been computed.
Took   0.222968936      seconds to compute.
Returning to main terminal...
Ready for next command.
```