Hands-on:

Thermoelectric and electronic transport properties with Wannier90+BoltzWann

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May 10, 2022

1 Outline

- Obtain MLWFs for the valence and low-lying conduction states of silicon.
- Calculate the electrical conductivity, the Seebeck coefficient and the thermal conductivity in the constant relaxation time approximation using the `BoltzWann` module[1, 2].

2 Input files & executables

- Directory: `wannier-tutorials/2022_05_Trieste/Fri.AM.Pizzi/`
- Input Files
  - `Si.scf`: The `pw.x` input file for ground state calculation
  - `Si.nscf`: The `pw.x` input file to obtain Bloch states on a uniform grid
  - `Si.pw2wan`: Input file for `pw2wannier90.x`
  - `Si.win`: The `wannier90.x` and `postw90.x` input file
- Executables:
  - `pw.x`, `pw2wannier90.x`, `wannier90.x`, and `postw90.x`
  - Available in `/media/ictpuser/AiiDA/bin/`

3 Steps

We will first run the standard Wannierization of silicon, then run the `postw90.x` with `BoltzWann` related parameters added to the input file.

1. Run `pw.x` to obtain the ground state of silicon

```
pw.x < Si.scf > scf.out
```

2. Run `pw.x` to obtain the Bloch states on a uniform k-point grid.

```
pw.x < Si.nscf > nscf.out
```

3. Run `wannier90.x` to generate a list of the required overlaps (written into the `Si.nnkp` file).

```
wannier90.x -pp Si
```

4. Run `pw2wannier90.x` to compute the overlap between Bloch states and the projections for the starting guess (written in the `Si.mmn` and `Si.amn` files).

```
pw2wannier90.x < Si.pw2wan > pw2wan.out
```

5. Run `wannier90.x` to compute the MLWFs.

```
wannier90.x Si
```

   Inspect the output file `Si.wout` and check if the convergence was reached both in the disentanglement and in the Wannierization steps. You may also want to plot the Wannier functions and the interpolated band structure.

6. Run `postw90.x` to calculate the transport coefficients.

```
# serial execution
postw90.x Si
# or parallel execution with, e.g. 4 MPI processes
mpirun -np 4 postw90.x Si
```

4 Analysis

- Inspect the output file `Si.wpout`. It summarizes the main details of the calculation (more details can be obtained by setting a larger value of the `iprint` flag). Check if no warnings are issued. Note that if no special flags are passed to `BoltzWann`, it assumes that the ab-initio calculation did not include magnetization effects, and thus it sets to 2 the number of electrons per state.
- Note also that the value of the relaxation time $\tau = 10\,\text{fs}$ in the example is set only as a representative value; note also that only the electrical and thermal conductivity depend on τ, while the Seebeck coefficient is independent of τ.
- Using your favorite plotting program, plot the `Si_boltzdos.dat` file to inspect the DOS, e.g. with `gnuplot`, see Fig. 1.

```
set xlabel 'E (eV)'
set ylabel 'DOS (ang^{-3})'
plot 'Si_boltzdos.dat' w l
```

- Using your favorite plotting program, plot columns 1 and 3 of the `Si_seebeck.dat` file to inspect the S_{xx} component of the Seebeck coefficient as a function of the chemical potential μ, at $T = 300\,\text{K}$. For example, with `gnuplot`, see Fig. 2.

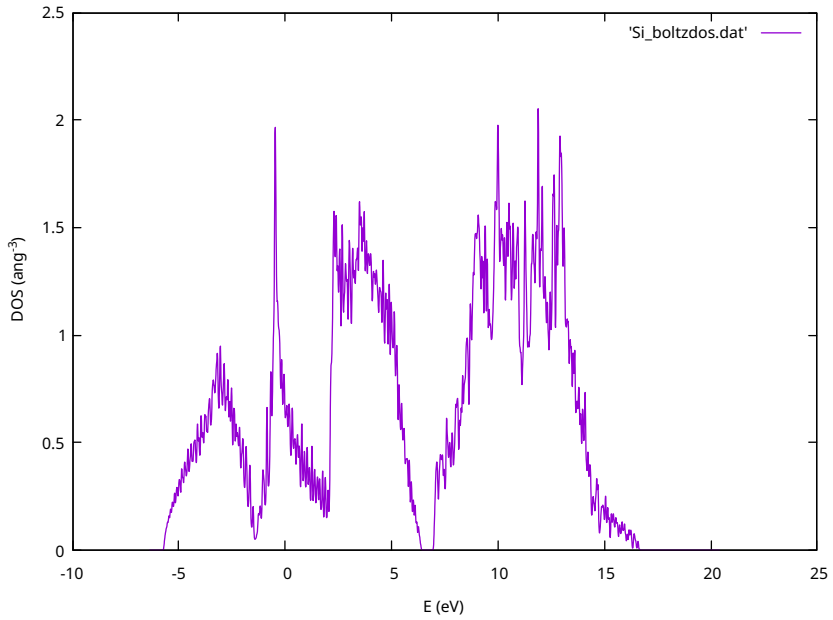

Figure 1: DOS of silicon using `BoltzWann` module.

```
set xlabel 'E (eV)'
set ylabel 'DOS (S_{xx} (V/K))'
plot 'Si_seebeck.dat' u 1:3 w l
```

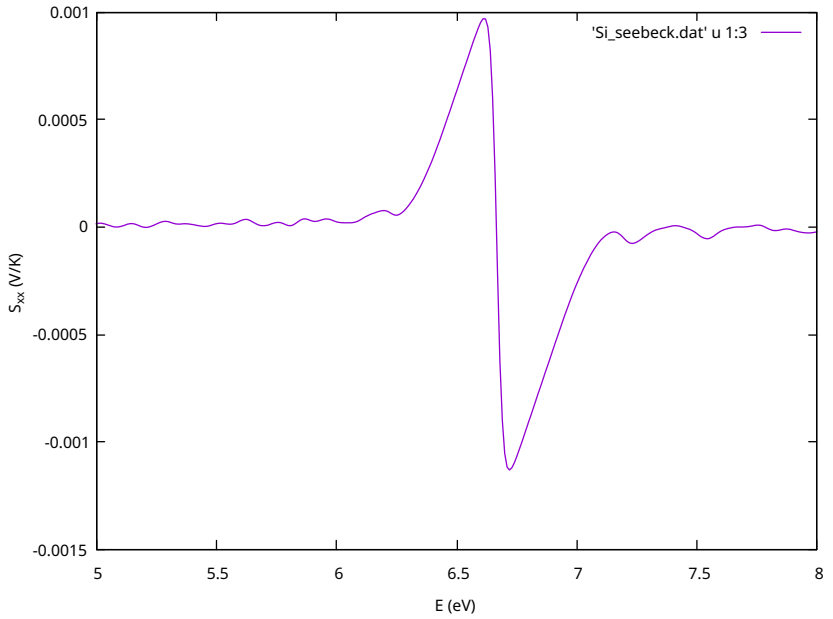

Figure 2: S_{xx} of silicon using `BoltzWann` module.

4.1 Further ideas

- Change the interpolation to a $60 \times 60 \times 60$ mesh and run again `postw90.x` to check if the results for the transport properties are converged.

- Change the `Si.win` input file so that it calculates the transport coefficients for temperatures from 300 K to 700 K, with steps of 200 K. Rerun `postw90.x` and verify that the increase in execution time is neglibile (in fact, most of the time is spent to interpolate the band structure on the k mesh).

  Plot the Seebeck coefficient for the three temperatures $T = 300\,\mathrm{K}$, $T = 500\,\mathrm{K}$ and $T = 700\,\mathrm{K}$. To do this, you have to filter the `Si_seebeck.dat` to select only those lines where the second column is equal to the required temperature. A possible script to select the S_{xx} component of the Seebeck coefficient for $T = 500\,\mathrm{K}$ using the `awk/gawk` command line program is the following:

  ```
  awk '{if ($2 == 500) {print $1, $3;}}' < Si_seebeck.dat \
      > Si_seebeck_xx_500K.dat
  ```

  Then, you can plot columns 1 and 2 of the output file `Si_seebeck_xx_500K.dat`.

- Try to calculate the Seebeck coefficient as a function of the temperature, for a $n-$doped sample with, e.g., $n = 1 \times 10^{18}\,\mathrm{cm}^{-3}$. Note that to this aim, you need to calculate consistently the value $\mu(T)$ of the chemical potential as a function of the temperature, so as to reproduce the given value of n. Then, you have to write a small program/script to interpolate the output of `BoltzWann`, that you should have run on a suitable grid of (μ, T) points.

References

[1] G. Pizzi, D. Volja, B. Kozinsky, M. Fornari, and N. Marzari, "BoltzWann: A code for the evaluation of thermoelectric and electronic transport properties with a maximally-localized Wannier functions basis", en, Comput. Phys. Commun. **185**, 422–429 (2014).

[2] G. Pizzi, D. Volja, B. Kozinsky, M. Fornari, and N. Marzari, "An updated version of BoltzWann: A code for the evaluation of thermoelectric and electronic transport properties with a maximally-localized Wannier functions basis", en, Comput. Phys. Commun. **185**, 2311–2312 (2014).