Exercise: Wannier Functions

We will construct maximally localized Wannier functions for $SrVO_3$ (or a material of your choice) using *wien2wannier* and *wannier90*.

NB: there is no w2web module for this. You have to use the command line.

NB2: Steps 1–8 will guide you through the complete "Wannierization" process. Everything after that is "optional".

More information:

`http://www.wien2k.at/reg_user/unsupported/wien2wannier/`
→ user guide

`http://wannier.org`

Easy as 1-2-3 . . .

1. standard Wien2k run
   - spacegroup 221 $Pm-3m$, $a = 7.2613$ Bohr
   - Sr $(0, 0, 0)$, V $(1/2, 1/2, 1/2)$, O $(0, 1/2, 1/2)$
   - obtain band structure[1]

2. identify target bands ("low-energy model")
   - minimal (d-only): V-t_{2g} around E_F
   - *or* (your choice) dp-model: V-t_{2g} + O-p

3. prepare a directory for wien2wannier
   - `prepare_w2wdir.sh` *case w2wdir*
     creates *w2wdir* and copies some files
   - cd *w2wdir*

[1] Do not use the `WIEN2k/SRC_templates/*.klist` files (old format, creates a problem at a later step); use *XCrysDen* to create a *case*`.klist`.

. . . 4-5-6-7-8

4. write input files: `init_w2w`
   - in `kgen`,
     - create a uniform mesh ($4 \times 4 \times 4$ is a good starting point)
     - do not shift k-mesh
   - follow instructions, using "common sense" . . .
5. eigenvectors on full k-mesh: `x lapw1`
6. compute overlap matrix: `w2w` *`case`*
7. set $E_F \leftarrow 0$: `shift_energy` *`case`*
8. optimize $U(\boldsymbol{k})$: `wannier90.x` *`case`*

. . . and you're done!

Consistency Checks and Analysis

- Wannier function spread $\langle \Delta \boldsymbol{r}^2 \rangle$
  - look for "Final State" in *case*`.wout`
  - should be $\sim 1.6\,\text{Å}^2$ for a *d*-only model
- compare band structure Wien2k vs. Wannier interpolation
  - in `gnuplot`:

```
plot 'case.spaghetti_ene' using ($4/0.53):5,
     'case_band.dat' with lines
```

- look at the hopping matrix elements
  ($\longleftrightarrow$ tight-binding Hamiltonian $H(\boldsymbol{R})$, *case*`_hr.dat`)
  - Do you see the proper symmetries?
  - Do the hoppings decay quickly enough?
    (Exponential localization!)

If You Still Have Time

- compare *d*-only and *dp*-models
  - How do the “V-*d*” WF change (hoppings, spread)?
- Check k-mesh convergence. When do you see convergence of
  - the band structure?
  - $H(\boldsymbol{R})$?
  - the spreads?
- plot the Wannier functions (→ user guide, or ask help)

1. `write_wplotin` *case*
2. `write_wplotdef` *case*
3. `prepare_plots.sh` *case*
4. `xsfAll.sh` *case*
5. `xcrysden -xsf` *case*`_`*i*`.xsf.gz`

- ...