Symmetry-adapted Wannier functions hands-on tutorial
Wannier 2022 Summer School

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PART I: SAWFs for the valence bands of GaAs

Outline: *Obtain symmetry-adapted Wannier functions out of four valence bands of GaAs, starting from several different initial conditions. For the theoretical background of the symmetry-adapted Wannier functions, see R. Sakuma, Phys. Rev. B* **87***, 235109 (2013).*

Directories: `SAWF_As_sp/`
`SAWF_Ga_p/`
`SAWF_Ga_s/`
`SAWF_Ga_sp/`
`MLWF_As_sp_Saddle/`
`pseudo/`

Within each directory you will also find a `ref/` *folder containing the reference input files for each calculation.*

Description of input files

- *DFT Input Files, common to all calculations*

  `GaAs.scf.in` *The* PWSCF *input file for ground state calculation*

  `GaAs.nscf.in` *The* PWSCF *input file to obtain Bloch states on a uniform grid*

- *Input Files, specific to each calculation. These can be found within each directory and might need to be modified depending on the calculation*

  `GaAs.pw2wan.in` *The input file for* `pw2wannier90`

  `GaAs.win` *The* `wannier90` *input file*

☞ STEP 1: Run DFT calculations

- *Run* PWSCF *to obtain the ground state density of GaAs*
  `$> pw.x < GaAs.scf.in > GaAs.scf.out`

- *Run* PWSCF *to obtain the Bloch states on a uniform k-point grid*
  `$> pw.x < GaAs.nscf.in > GaAs.nscf.out`

☞ STEP 2: Compute SAWFs from *s*-like and *p*-like orbitals centred on the As atom

Outline: Symmetry-adapted mode: one s-like and three p-like Wannier functions centered at As

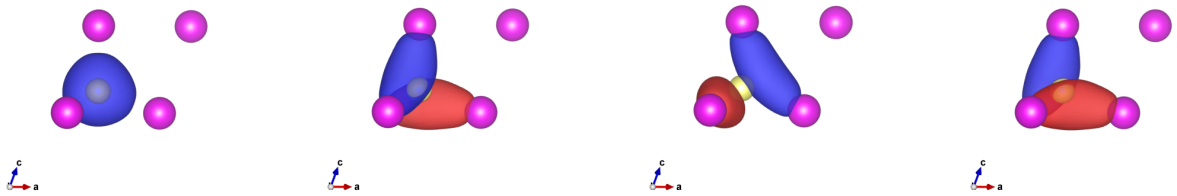
- *cd into* `SAWF_As_sp/`

- *Check the additional parameters for the symmetry-adapted mode in* `GaAs.win` *and* `GaAs.pw2wan.in`
- *Run* `wannier90` *to generate a list of the required overlaps (written into the* `GaAs.nnkp` *file).*
  `$> wannier90.x -pp GaAs`
- *Run* `pw2wannier90` *to compute the overlap between Bloch states, the projections for the starting guess, and the symmetry information needed for symmetry-adapted mode written in the* `GaAs.mmn`*,* `GaAs.amn`*, and* `GaAs.dmn` *files, respectively. Additionally* `GaAs.sym` *file is also created.*
  `$> pw2wannier90.x < GaAs.pw2wan.in > GaAs.pw2wan.out`
- *Run* `wannier90` *to compute the SAWFs.*
  `$> wannier90.x GaAs`
- *Compare the results for a* $4 \times 4 \times 4$ *k-point sampling with those in Table I in "R. Sakuma, Phys. Rev. B 87, 235109 (2013)", which we report here. See also* `ref/` *directory, in which one can find the input files (*`GaAs.win` *and* `GaAs.pw2wan.in`*) and an output file (*`GaAs.wout`*).*

Ω_I	Ω_D	Ω_{OD}	Ω	Ω_n	
				s	p
6.124	0.012	3.502	9.639	1.450	2.730

Table 1: Spreads of the four As-centered symmetry adapted Wannier functions of GaAs in Å calculated with $4 \times 4 \times 4$ k-point sampling. Ω_I denotes the gauge-independent part of the total spread functional Ω, Ω_D denotes the diagonal part, Ω_{OD} the off-diagonal part and Ω_n denotes the spread of one Wannier function.

- *Plot the SAWFs using xcrysden.*
  `$> xcrysden --xsf GaAs_0000*.xsf`



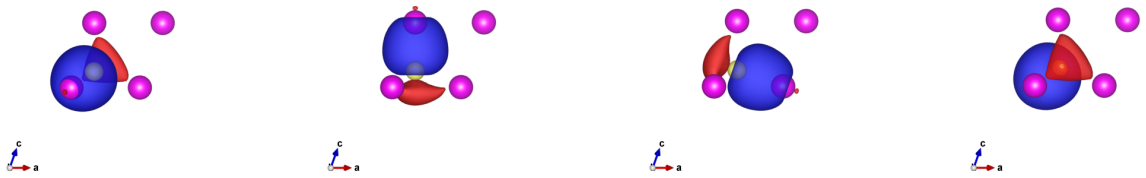
(a) s-like (b) p-like (c) p-like (d) p-like

Figure 1: Four SAWFs from a) one s-like orbital and b)-d) three p-like orbitals centred on the As atom as initial projections. Ga atoms are represented by pink spheres and As atoms by yellow spheres. Isosurface value set to ± 1.0 Å$^{-3/2}$.

☞ STEP 3 (optional): Compute MLWFs from s-like and p-like orbitals centred on the As atom + small perturbation

Outline: Maximally-localized Wannier functions starting from As-atomic-centered projections (+ small perturbation)

- *cd into* `MLWF_As_sp_Saddle/`
- *Modify* `GaAs.win` *to turn off symmetry-adapted mode. Comment out the following two lines in* `GaAs.win`
  ```
  site_symmetry = .true.
  symmetrize_eps= 1d-9
  ```
- *Modify* `GaAs.pw2wan.in` *to turn off symmetry-adapted mode by setting*
  `write_dmn = .false.`
- *Put small perturbation to the center(s) of the initial projection(s).*
- *Run* `wannier90` *to generate a list of the required overlaps (written into the* `GaAs.nnkp` *file).*
  ```
  $> wannier90.x -pp GaAs
  ```
- *Run* `pw2wannier90` *to compute the overlap between Bloch states and the projections for the starting guess written in the* `GaAs.mmn` *and* `GaAs.amn` *files, respectively.*
  ```
  $> pw2wannier90.x < GaAs.pw2wan.in > GaAs.pw2wan.out
  ```
- *Run* `wannier90` *to compute the MLWFs.*
  ```
  $> wannier90.x GaAs
  ```
- *Compare the results with those in* `../SAWF_As_sp`.
- *Plot the MLWFs using xcrysden.*
  ```
  $> xcrysden --xsf GaAs_0000*.xsf
  ```



(a) sp^3-like (b) sp^3-like (c) sp^3-like (d) sp^3-like

Figure 2: Four MLWFs for valence bands in GaAs, starting from a) one s-like and b)-d) three p-like orbitals centred slightly off the As atom. Ga atoms are represented by pink spheres and As atoms by yellow spheres. Isosurface value set to ± 1.0 Å$^{-3/2}$.

☞ STEP 4: Compute SAWFs from s-like and p-like orbitals centred on the Ga atom

Outline: Symmetry-adapted mode: one s-like and three p-like Wannier functions centered at Ga

- *cd into* `SAWF_Ga_sp/`
- *Set* `num_wann=4` *and fill out the projection part in* `GaAs.win`.

- *Modify* `GaAs.win` *to turn on symmetry-adapted mode. Uncomment the following two lines in* `GaAs.win`
  ```
  !site_symmetry = .true.
  !symmetrize_eps= 1d-9
  ```

- *Modify* `GaAs.pw2wan.in` *to turn on symmetry-adapted mode by setting* `write_dmn=.true.`

- *Run* `wannier90` *to generate a list of the required overlaps (written into the* `GaAs.nnkp` *file).*
  ```
  $> wannier90.x -pp GaAs
  ```

- *Run* `pw2wannier90` *to compute the overlap between Bloch states, the projections for the starting guess, and the symmetry information needed for symmetry-adapted mode written in the* `GaAs.mmn`, `GaAs.amn`, *and* `GaAs.dmn` *files, respectively. Additionally* `GaAs.sym` *file is also created.*
  ```
  $> pw2wannier90.x < GaAs.pw2wan.in > GaAs.pw2wan.out
  ```

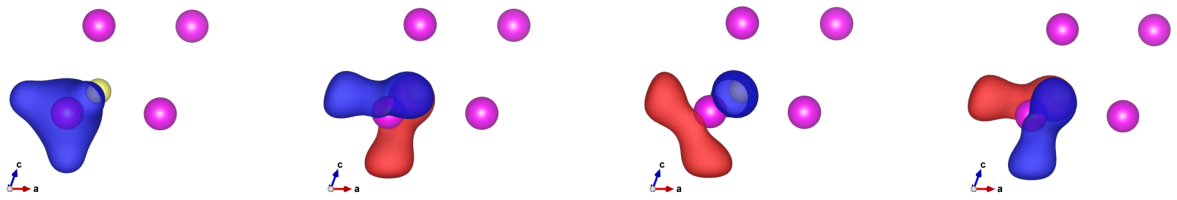
- *Run* `wannier90` *to compute the SAWFs.*
  ```
  $> wannier90.x GaAs
  ```

- *Compare the results for a* $4 \times 4 \times 4$ *k-point sampling with those in Table I in "R. Sakuma, Phys. Rev. B 87, 235109 (2013)", which we report here. See also* `ref/` *directory, in which one can find the input files (*`GaAs.win` *and* `GaAs.pw2wan.in`*) and an output file (*`GaAs.wout`*).*

Ω_I	Ω_D	Ω_{OD}	Ω	Ω_n	
				s	p
6.124	0.151	7.648	13.924	2.448	3.825

Table 2: Spreads of the four Ga-centered symmetry adapted Wannier functions of GaAs in Å calculated with $4 \times 4 \times 4$ k-point sampling. See caption in Tab. 1 for definition of symbols.

- *Plot the SAWFs using xcrysden.*
  ```
  $> xcrysden --xsf GaAs_0000*.xsf
  ```



(a) s-like (b) p-like (c) p-like (d) p-like

Figure 3: Four SAWFs from a) one s-like orbital and b)-d) three p-like orbitals centred on the Ga atom as initial projections. Ga atoms are represented by pink spheres and As atoms by yellow spheres. Isosurface value set to ± 1.0 Å$^{-3/2}$.

☞ STEP 5: Compute SAWFs from one s-like orbital centered on the Ga atom

Outline: Symmetry-adapted mode: one s-like Wannier function centered at Ga

- *cd into* `SAWF_Ga_s/`
- *Set* `num_wann=1` *and fill out the projection part in* `GaAs.win`.
- *Modify* `GaAs.win` *to turn on symmetry-adapted mode. Uncomment the following two lines in* `GaAs.win`
  ```
  !site_symmetry = .true.
  !symmetrize_eps= 1d-9
  ```
- *Modify* `GaAs.pw2wan.in` *to turn on symmetry-adapted mode by setting* `write_dmn=.true.`
- *Run* `wannier90` *to generate a list of the required overlaps (written into the* `GaAs.nnkp` *file).*
  ```
  $> wannier90.x -pp GaAs
  ```
- *Run* `pw2wannier90` *to compute the overlap between Bloch states, the projections for the starting guess, and the symmetry information needed for symmetry-adapted mode written in the* `GaAs.mmn`, `GaAs.amn`, *and* `GaAs.dmn` *files, respectively. Additionally* `GaAs.sym` *file is also created.*
  ```
  $> pw2wannier90.x < GaAs.pw2wan.in > GaAs.pw2wan.out
  ```
- *Run* `wannier90` *to compute the SAWF.*
  ```
  $> wannier90.x GaAs
  ```
- *Plot bands.*
  ```
  $> gnuplot
  gnuplot> load "GaAs_band.gnu"
  gnuplot> replot "../DFT_band.dat" w l lt -1, "GaAs_band.dat" lt 1
  ```
  See also `ref/` *directory, in which one can find the input files (*`GaAs.win` *and* `GaAs.pw2wan.in`*) and an output file (*`GaAs.wout`*)*
- *Compare the results with those in Figure 1 and Table I in "R. Sakuma, Phys. Rev. B 87, 235109 (2013)".*
- *Plot the SAWF using xcrysden.*
  ```
  $> xcrysden --xsf GaAs_00001.xsf
  ```

☞ STEP 6: Compute SAWFs from three p-like orbitals centred on the Ga atom

Outline: Symmetry-adapted mode: three p-like Wannier functions centered at Ga

- *cd into* `SAWF_Ga_p/`
- *Set* `num_wann=3` *and fill out the projection part in* `GaAs.win`.
- *Modify* `GaAs.win` *to turn on symmetry-adapted mode. Uncomment the following two lines in* `GaAs.win`
  ```
  !site_symmetry = .true.
  !symmetrize_eps= 1d-9
  ```
- *Modify* `GaAs.pw2wan.in` *to turn on symmetry-adapted mode by setting* `write_dmn=.true.`

- *Run* `wannier90` *to generate a list of the required overlaps (written into the* `GaAs.nnkp` *file).*
  `$> wannier90.x -pp GaAs`

- *Run* `pw2wannier90` *to compute the overlap between Bloch states, the projections for the starting guess, and the symmetry information needed for symmetry-adapted mode written in the* `GaAs.mmn`*,* `GaAs.amn`*, and* `GaAs.dmn` *files, respectively. Additionally* `GaAs.sym` *file is also created.*
  `$> pw2wannier90.x < GaAs.pw2wan.in > GaAs.pw2wan.out`

- *Run* `wannier90` *to compute the SAWFs.*
  `$> wannier90.x GaAs`

- *Plot bands.*
  ```
  $> gnuplot
  gnuplot> load "GaAs_band.gnu"
  gnuplot> replot "../DFT_band.dat" w l lt -1, "GaAs_band.dat" lt 1
  ```
  See also `ref/` *directory, in which one can find the input files (*`GaAs.win` *and* `GaAs.pw2wan.in`*) and an output file (*`GaAs.wout`*)*

- *Compare the results with those in Figure 1 and Table I in "R. Sakuma, Phys. Rev. B 87, 235109 (2013)".*

- *Plot the SAWFs using xcrysden.*
  `$> xcrysden --xsf GaAs_0000*.xsf`

PART II: SAWFs for Cu

Outline: Compute symmetry-adapted Wannier functions for Cu. By symmetry-adapted mode, for example, we can make atomic centered s-like Wannier function, which is not possible in the usual procedure to create maximally localized Wannier functions. For the theoretical background of the symmetry-adapted Wannier functions, see R. Sakuma, Phys. Rev. B **87***, 235109 (2013).*

- **Directories:** `pseudo/`

Description of input files

- *DFT Input Files, common to all calculations*

  `Cu.scf.in` *The* PWSCF *input file for ground state calculation*

  `Cu.nscf.in` *The* PWSCF *input file to obtain Bloch states on a uniform grid*

- *Input Files, specific to each calculation. These might need to be modified depending on the calculation*

  `Cu.pw2wan.in` *The input file for* `pw2wannier90`

  `Cu.sym` `pw2wannier90` *reads this file when* ‘`read_sym = .true.`’ *in* `Cu.pw2wan.in`*. By default,* ‘`read_sym = .false.`’ `and Cu.sym is the output of pw2wannier90`*, in which the symmetry operations employed in the calculation are written for reference.*

  `Cu.win` *The* `wannier90` *input file*

☞ STEP 1: Run DFT calculations

- *Run* PWSCF *to obtain the ground state of Cu*
  `pw.x < Cu.scf.in > Cu.scf.out`
- *Run* PWSCF *to obtain the Bloch states on a uniform k-point grid*
  `pw.x < Cu.nscf.in > Cu.nscf.out`

☞ STEP 2: Compute SAWFs for Cu from five *d*-like orbitals centred on Cu and one *s*-like orbital centred in the interstitial site

Outline: Symmetry-adapted Wannier functions for Cu (s-like Wannier function centered at (1/4,1/4,1/4) + atomic-centered d-like Wannier functions)

- *Modify* `Cu.win` *to turn on symmetry-adapted mode. Uncomment the following two lines in Cu.win*
  ```
  !site_symmetry = .true.
  !symmetrize_eps= 1d-9
  ```
- *Modify* `Cu.pw2wan.in` *to turn on symmetry-adapted mode by setting*
  `write_dmn=.true.`
- *Modify* `Cu.pw2wan.in` *to use customized symmetry operations compatible with site-symmetry group at (1/4,1/4,1/4). N.B. inversion symmetry needs to be removed! In* `Cu.pw2wan.in` *set*
  `read_sym=.true.` *(then* `pw2wannier.x` *will require* `Cu.sym`*)*
- *Prepare* `Cu.sym` *file.*
  `$> cp ../GaAs/SAWF_As_sp/GaAs.sym Cu.sym` *(symmetry operations taken from the GaAs example. N.B. GaAs does not have inversion symmetry!)*
- *Run* `wannier90` *to generate a list of the required overlaps (written into the* `Cu.nnkp` *file).*
  `wannier90.x -pp Cu`
- *Run* `pw2wannier90` *to compute the overlap between Bloch states, the projections for the starting guess, and the symmetry information needed for symmetry-adapted mode (written in the* `Cu.mmn`*,* `Cu.amn`*, and* `Cu.dmn` *files, respectively).*
  `pw2wannier90.x < Cu.pw2wan.in > Cu.pw2wan.out`
- *Run* `wannier90` *to compute the SAWFs.*
  `wannier90.x Cu`
- *Plot bands.*
  ```
  $> gnuplot
  gnuplot> load "Cu_band.gnu"
  gnuplot> replot "DFT_band.dat" w l lt -1, "Cu_band.dat" lt 1
  ```
  See also ref directory, in which one can find the input files (`Cu.win` *and* `Cu.pw2wan.in`*) and an output file (*`Cu.wout`*)*
- *Compare the results with those in Fig.3 and Table II in "R. Sakuma, Phys. Rev. B 87, 235109 (2013)", which we report here*

Energy window [E_f -10 (eV): E_f +10 (eV)]						
Ω_I	Ω_D	Ω_{OD}	Ω	Ω_n		
				s	t_{2g}	e_g
3.968	0.107	0.511	4.587	2.042	0.534	0.471

Table 3: Spreads of six symmetry adapted Wannier functions (from one s-like + five d-like oribtals) in Cu in Å calculated with $8 \times 8 \times 8$ k-point sampling. See caption in Tab. 1 for definition of Ω symbols. From crystal field theory we know that the 5 d orbitals split into two sets (3+2). t_{2g} is the Mulliken symbol for the three-fold degenerate subspace. e_g is the Mulliken symbol for the doubly-degenerate subspace.

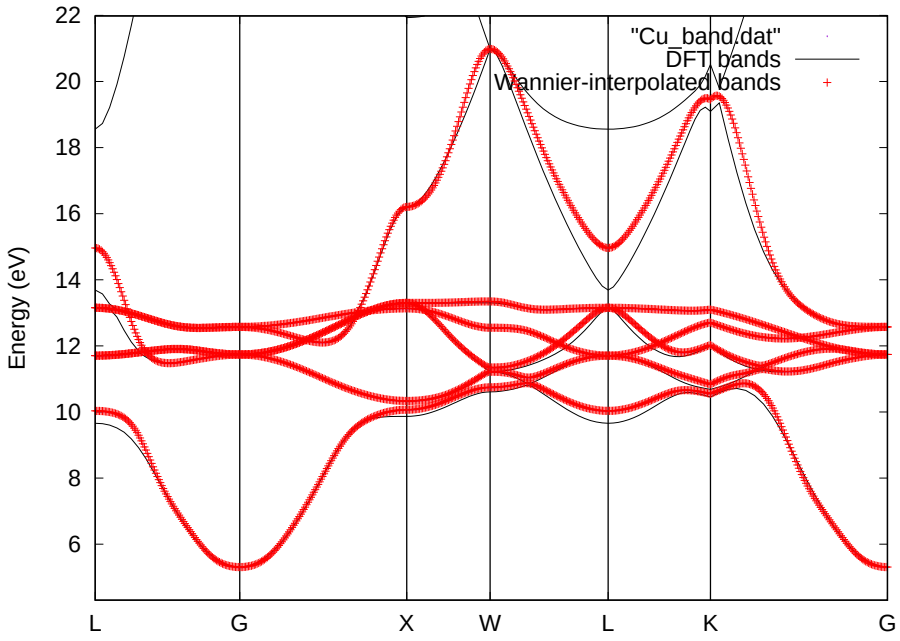
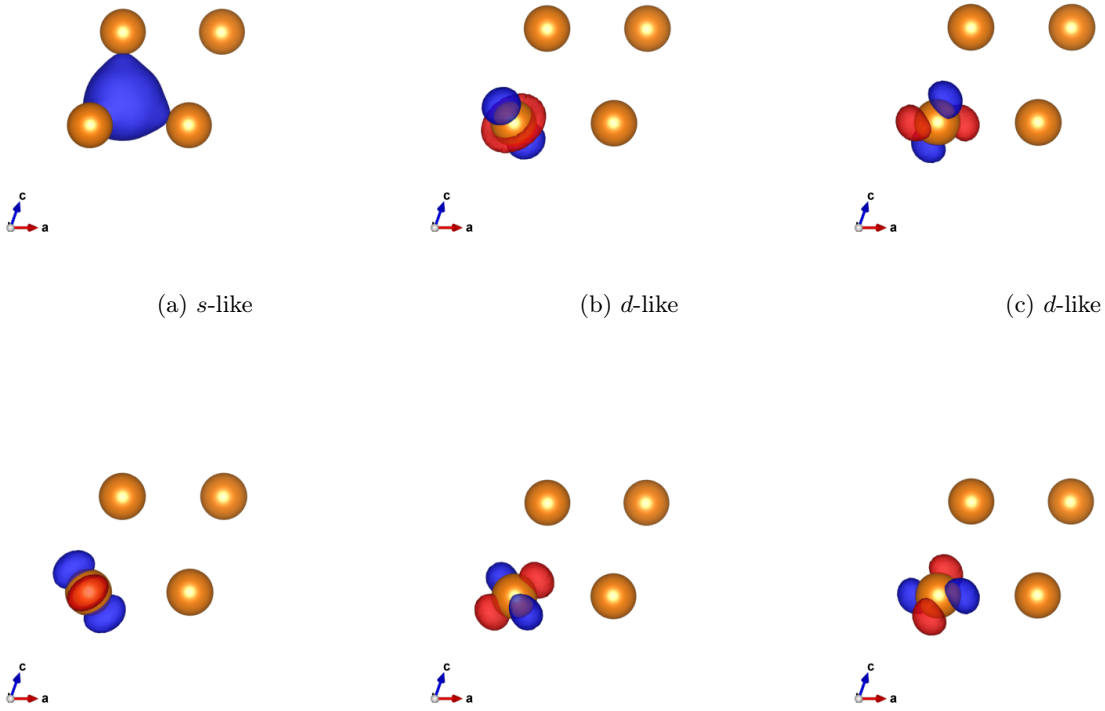


Figure 4: Bandstructure of Cu. DFT bands (solid lines), Wannier-interpolated bands (red plus).

► *Plot the SAWFs using xcrysden.*
```
$> xcrysden --xsf Cu_0000*.xsf
```

✍ *Change the upper bound of the disentanglement window as E_f + 20 (eV) and leave the lower bound equal to E_f - 10 (eV) and recompute the bandstructure and the SAWFs.*



(a) *s*-like (b) *d*-like (c) *d*-like

(d) *d*-like (e) *d*-like (f) *d*-like

Figure 5: Six SAWFs from a) one *s*-like orbital and b)-f) 5 *d*-like orbitals centred on the Cu atom as initial projections. Cu atoms are represented by orange spheres. Isosurface value set to ± 1.0 Å$^{-3/2}$.

PART III: SAWFs for H_3S

Outline: Compute symmetry-adapted Wannier functions for H_3S. For the theoretical background of the symmetry-adapted Wannier functions, see R. Sakuma, Phys. Rev. B **87**, *235109 (2013).*

- **Directories:** `MLWF_12band/`
  `SAWF_12band/`
  `SAWF_7band/`
  `pseudo/`

Description of input files

- *DFT Input Files, common to all calculations*

  `H3S.scf.in` *The* PWSCF *input file for ground state calculation*

  `H3S.nscf.in` *The* PWSCF *input file to obtain Bloch states on a uniform grid*

- *Input Files, specific to each calculation. These can be found within each directory and might need to be modified depending on the calculation*

  `H3S.pw2wan.in` *The input file for* `pw2wannier90`

  `H3S.win` *The* `wannier90` *input file*

☞ STEP 1: Run DFT calculations

- *Run* PWSCF *to obtain the ground state of* H_3S
  `pw.x < H3S.scf.in > H3S.scf.out`
- *Run* PWSCF *to obtain the Bloch states on a uniform k-point grid*
  `pw.x < H3S.nscf.in > H3S.nscf.out`

☞ STEP 2: Compute MLWFs for H_3S for 12 bands

Outline: Maximally-localized Wannier functions: H_3S*, 12 band model*

- *Run* `wannier90` *to generate a list of the required overlaps (written into the* `H3S.nnkp` *file).*
  `wannier90.x -pp H3S`
- *Run* `pw2wannier90` *to compute the overlap between Bloch states and the projections for the starting guess (written in the* `H3S.mmn` *and* `H3S.amn` *files, respectively).*
  `pw2wannier90.x < H3S.pw2wan.in > H3S.pw2wan.out`
- *Run* `wannier90` *to compute the MLWFs.*
  `wannier90.x H3S`
- *Check Wannier centers and spreads (see* `H3S.wout`*).*
- *Plot bands.*
  ```
  $> gnuplot
  gnuplot> load "H3S_band.gnu"
  gnuplot> replot "../DFT_band.dat" w l lt -1, "H3S_band.dat" lt 1
  ```
  See also ref directory, in which one can find the input files (`H3S.win` *and* `H3S.pw2wan.in`*) and an output file (*`H3S.wout`*)*

☞ STEP 2: Compute SAWFs for H_3S for 12 bands

Outline: Symmetry-adapted Wannier functions: H_3S*, 12 band model*

- *Modify* `H3S.win` *to turn on symmetry-adapted mode. Uncomment the following two lines in Cu.win*
  ```
  !site_symmetry = .true.
  !symmetrize_eps= 1d-9
  ```
- *Modify* `H3S.pw2wan.in` *to turn on symmetry-adapted mode by setting*
  `write_dmn=.true.`
- *Run* `wannier90` *to generate a list of the required overlaps (written into the* `H3S.nnkp` *file).*
  `wannier90.x -pp H3S`
- *Run* `pw2wannier90` *to compute the overlap between Bloch states, the projections for the starting guess, and the symmetry information needed for symmetry-adapted mode (written in the* `H3S.mmn`*,* `H3S.amn`*, and* `H3S.dmn` *files, respectively).*
  `pw2wannier90.x < H3S.pw2wan.in > H3S.pw2wan.out`
- *Run* `wannier90` *to compute the SAWFs.*
  `wannier90.x H3S`

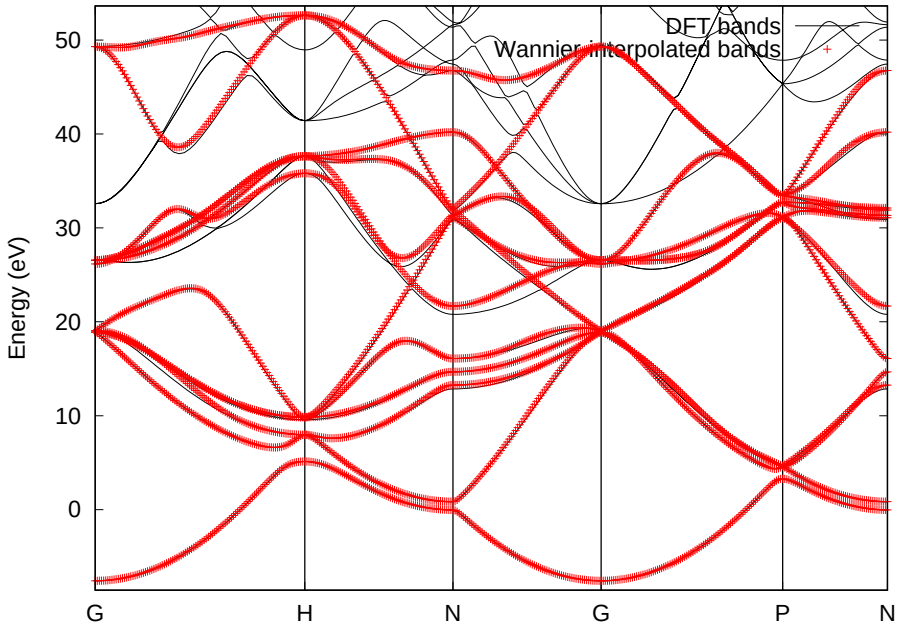


Figure 6: Bandstructure of H_3S. DFT bands (solid lines), Wannier-interpolated bands (red plus).

- *Check Wannier centers and spreads (see* `H3S.wout`*) & Compare the results with those in* `"../MLWF_12band/"`.
- *Plot bands.*
```
$> gnuplot
gnuplot> load "H3S_band.gnu"
gnuplot> replot "../DFT_band.dat" w l lt -1, "H3S_band.dat" lt 1
```

☞ STEP 3: Compute SAWFs for H_3S for 7 bands

Outline: Symmetry-adapted Wannier functions: H_3S, 7 band model (atomic-centered s-like orbital at H and atomic-centered s-like and p-like orbitals at S)

- *Set* `num_wann=7` *and fill out the projection part in* `H3S.win`.
- *Modify* `H3S.win` *to turn on symmetry-adapted mode. Uncomment the following two lines in* `H3S.win`
```
!site_symmetry = .true.
!symmetrize_eps= 1d-9
```
- *Modify* `H3S.pw2wan.in` *to turn on symmetry-adapted mode by setting* `write_dmn=.true.`
- *Run* `wannier90` *to generate a list of the required overlaps (written into the* `H3S.nnkp`*).*
```
$> wannier90.x -pp H3S
```
- *Run* `pw2wannier90` *to generate* `H3S.amn`, `H3S.mmn`, `H3S.dmn`, *and* `H3S.eig` *files (additionally* `H3S.sym` *file is also created).*
```
$> pw2wannier90.x < H3S.pw2wan.in > H3S.pw2wan.out
```

- *Run* `wannier90` *to construct SAWFs.*
  ```
  $> wannier90.x H3S
  ```
- *Check Wannier centers and spreads (see* `H3S.wout`*).*
- *Plot bands.*
  ```
  $> gnuplot
  gnuplot> load "H3S_band.gnu"
  gnuplot> replot "../DFT_band.dat" w l lt -1, "H3S_band.dat" lt 1
  ```