Transformation of Wannier90 data to $\mathcal{AMULET}$ format

The ***wannier2amulet*** routine is designed to convert a real space Hamiltonian obtained by the Wannier90 program to $\mathcal{AMULET}$ format. At this point one assume that you have already converged a self-consistent calculation with a band structure package of your choice and have constructed maximally-localized Wannier functions (MLWF) (see N. Marzari, D. Vanderbilt, PRB **56**, 12847 (1997).

To obtain the Hamiltonian in **k**-space in the $\mathcal{AMULET}$ format one needs to have next input file(s):

- ***hrup.ini*** – can be copied from `seedname_hr.dat` file
- ***hrdn.ini*** – in case of a spin-polarized calculation
- ***klist.ini*** – an optional file that contains **k**-points coordinates.

In case of use of the WIEN2k package and its Wien2wannier interface the above mentioned files will automatically have proper names.

The ***klist.ini*** is the optional file with a simple format shown below.

```
 0.000000000  0.000000000  0.000000000
 0.000000000  0.000000000  0.125000000
 0.000000000  0.000000000  0.250000000
 0.000000000  0.000000000  0.375000000
 0.000000000  0.000000000  0.500000000
 0.000000000  0.000000000  0.625000000
 0.000000000  0.000000000  0.750000000
 0.000000000  0.000000000  0.875000000
 0.000000000  0.125000000  0.000000000
 0.000000000  0.125000000  0.125000000
 .....
```

If the ***wannier2amulet*** routine will not find this file, it will prompt for a division along different directions of **k**-space.

In case of successful execution of ***wannier2amulet*** you will find a ***hamilt.am*** file with the Hamiltonian written in the $\mathcal{AMULET}$ format.