Wannier90 3.0 Workshop SCDM Tutorial

This tutorial is divided into two parts, one for valence bands and one for valence and conduction bands. Example 27 in the `Wannier90` documentation provides additional information and an analogous example with Silicon.

Isolated bands

First, we will consider a simple system and use the SCDM implementation in `Wannier90` to construct localized basis functions. The files may be found in the `isolated` directory.

1. First, run a SCF and NSCF calculation with QE via

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

   followed by

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

2. Now, fill in the missing information in the `GaAs.win` and `GaAs.pw2wan` files. This will require adding the necessary snippet in the `.win` file to tell `Wannier90` to use automated projections and the keywords in the `.pw2wan` file to set up the "isolated" case. The keywords may be found in the `Wannier90` documentation and were outlined in the talk. After this is completed you may proceed with using `Wannier90` to generate localized basis functions as

   ```
   wannier90.x -pp GaAs
   ```

   followed by

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

   and finally

   ```
   wannier90.x GaAs
   ```

3. To explore the SCDM implementation try varying the number of iterations you let `Wannier90` run for and compare the spread along with the visual character of the local functions. You may also want to try using random projections as an initial guess, what differences do you see?

Valence and conduction bands

Now, we will consider using the SCDM implementation for entangled bands; once again for GaAs. The files for this part of the turorial are in `erfc`.

1. First, run a SCF and NSCF calculation with QE via

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

followed by

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

2. Now, fill in the missing information in the `GaAs.win` and `GaAs.pw2wan` files. This will require adding the necessary snippet in the `.win` file to tell `Wannier90` to use automated projections and the keywords in the `.pw2wan` file to set up the "erfc" case with $\mu = 11$ and $\sigma = 4$ (or pick your own parameters—you could try slight variations to see how sensitive the results are). The keywords may be found in the `Wannier90` documentation and were outlined in the talk.

3. To explore the SCDM implementation try varying the number of iterations you let `Wannier90` run for (both the disentanglement and the localization) and compare the spread along with the visual character of the local functions. As before, you could try using random projections as an initial guess, what differences do you see?

4. Does the generated band structure plot match your expectations?