

Density functional theory of crystals with FPLO - Wannier functions and tight binding

Tutorial at the QUANTY workshop in Heidelberg

Tuesday 24th September, 2024

This is a set of tutorials we will (partially) discuss during the QUANTY workshop in Heidelberg. Once you have finished these examples you can have a look at the folder [FPLO_SomeExamples] and [FPLO_SomeExamples_with_results]. One can use QUANTY scripts to run FPLO calculations to self consistency and create the Wannier orbitals and a tight binding representation of the bandstructure. Note that the newer version of FPLO (21 and beyond) allow one to script in Python as well. This is very powerful and useful. Have a look at the documentation or discuss among each other on how to do this.

In this task we will calculate the (atomic like) Wannier functions and tight binding Hamiltonian of NiO. At the end of the tutorial you should be able to reproduce Fig 2 and Fig 11 of PRB 85, 165113, Multiplet ligand-field theory using Wannier orbitals.

1 DFT self consistent potential

In order to calculate the Wannier functions and tight binding Hamiltonian we first need to calculate the DFT potentials. For this we do a full DFT calculation of NiO including a calculation of the density of states and bands and look at the band character.

- (i) Obtain the experimental crystal structure of NiO from the ICSD data base. <https://icsd.fiz-karlsruhe.de> in the field Composition under Chemistry type "Ni O" in the field Number of Elements type "2". NiO has a cubic rock-salt structure, which at low temperatures gets a slight trigonal distortion. We are going to neglect the trigonal distortion and aim for the cubic rock-salt (NaCl like) structure.
- (ii) Create a new directory (NiO) and initialize the calculation with fedit. Use the standard LDA functional and about 40 k-points per direction.
- (iii) Run the potential to self consistency
- (iv) calculate the DFT band-structure and density of states
- (v) include the band-character and identify the O-p and Ni-d like bands.

2 Ni only Wannier functions

Once we have the DFT solutions we can generate the Wannier functions. The Wannier functions are a Fourier transform of a set of bands. In order to do the Fourier transform we need to indicate which bands to include. Furthermore we need to pick a phase of the band eigen-functions. This we do by identifying a set of atomic basis functions to which we project.

The input to generate the Wannier functions in FPLO is done by adding the file `"=.wandef"` to the FPLO folder. In this file the needed definitions are made, defining the energy window for the bands we use in the Fourier transform as well as the orbitals to project on and some other settings.

- (i) Copy the file `"=.wandef"` provided as example to the DFT directory where you are working. Open the file with a text editor and with the use of the FPLO manual see if you understand the input.
- (ii) run `fplo`. This will generate the projections. Pipe the output to the file `out.wandef`
- (iii) run `fplo` again. This will generate the Wannier functions and band-structure. Pipe the output to the file `out.wan`
- (iv) plot the Wannier bands and the full DFT bands on top of each other.
- (v) Look at the hopping matrix elements for the tight binding model (file `out.wan`). Determine the dispersion of the z^2 orbital along the k_z direction.
- (vi) Besides the tight binding model FPLO also returns the Wannier functions on a grid. plot the Wannier functions. For this you can use `xfplo`.

3 Ni and O Wannier functions

Expand the previous calculation to include both the Ni-3d orbitals and O-2p orbitals.

- (i) Determine the O-O values of $pp\pi$ and $pp\sigma$ as well as the Ni-O values of $pd\pi$ and $pd\sigma$.
- (ii) Discuss how atomic like the Wannier functions are, both for the Ni-3d orbitals and the O-2p orbitals. Also discuss why they deviate.