# Wannier90 v3.0 school, Virtual Edition 2020

## Speaker: QuanSheng Wu

### 25 March 2020 - Questions and answers session

- **How is it possible that Wannier Tools does not need the .spn file?**
    - WannierTools assumes that the basis elements are orthogonal with each other. WannierTools assumes also that the WF basis elements are pure spin-up and spin-down. If there is a mixture of spin-up and spin-down in the WFs, especially when you are using MLWF, then WannierTools can't get trustable results.
- **How can one define hybrid Wannier functions? Are they different from normal Wannier functions?**
    - Hybrid Wannier functions (HWF) are defined as a Fourier transform of the Bloch wave functions in one direction, but they keep the momentum *k* along the other two directions unchanged. Instead, normal Wannier functions are the Fourier transform of Bloch wave functions in all three directions.
- **To find the Chern number one needs to break symmetry-inversion. So is it important to consider spin-orbit coupling?**
    - Chern number requires the breaking of time-reversal symmetry. However, it's not necessary to consider spin-orbit coupling to get the Chern number. One example is the quantum Hall effect which only requires a magnetic field.
- **With multiple bands, how is it possible to define a Chern number for each band?**
    - The Chern number is only defined for an isolated band or isolated group of bands. If a group of bands is isolated from the other bands, the Chern number can be defined as the trace of integral of non-Abelian Berry curvature.
- **Calculate for a particular nodal line?**
    - WannierTools can find the nodal line of a given tight-binding model if there is.
- **Is there a connection between the Berry curvature and the magnetic anisotropy energy (MAE), since MAE depends in many systems on the orbital magnetization like in FeCo alloy?**
    - I am not sure there is such a connection.
- **Can you say a few words on the interface between WannierTools and W90?**
    - WannierTools can read the tight-binding model file "wannier90_hr.dat" from W90. The tight-binding model file should be in the same format as that of W90 if prepared manually by the user.
- **There is some redundancy in the input to WannierTools, can this be improved? Moreover, can the input text use the same format as the output, so one can copy-paste and it's easier?**

    - Thanks for the suggestion. It should be improved in the future.
- **How to choose NumOccupied? I found that you have mentioned NumOccupied to be 1 in most of wt.in file.**
    - Please refer to http://www.wanniertools.com/input.html#system
- **When you calculate the hybrid WFs in WannierTools, what assumptions do you make about the WFs that make the TB model?**
    - The assumptions are the same as that of WannierTools:
        - The basis elements are orthogonal
        - Tight-binding approximation, i.e., the basis is taken as Delta function.
        - The basis set is complete
- **Does WannierTools use only atomic-like orbitals? Or it is just for symmetry.**
    - WannierTools works fine with the above three conditions for general properties. If you want to calculate some symmetry protected properties, then you need to use symmetrized WFs or atomic-like orbitals of which the Hamiltonian can be symmetrized with a symmetrization tool in our package.
- **Do we need all cards like SURFACE for bulk calculations such as finding Weyl points?**
    - Until WannierTools v2.5.1, the answer is yes. We need to set NumOccupied and the SURFACE card for all functionalities no matter if you are using it or not. It will be improved in the future.
- **If importing a TB model from W90, the PROJECTORS in the wt.in need to correspond to the symmetry of the MLWFs used to generate the TB model, correct? So the WFs should be atomic-like?**
    - The projectors name should be like this: “s”, “pz”, “px”, “py”, “dz2”, “dxz”, “dyz”, “dx2-y2”, “dxy”. However, until v2.5.1, The name of the projectors is not used. So you can always use “s” orbital as the name of a projector. However, the number of names should be consistent with the number of projectors. For example, if you constructed ‘sp3’ orbitals, then you need to write four ‘s’ orbitals.
- **Do we need to specify SURFACE for bulk calculations?**
    - Yes, we need to specify it although we don't use it in WannierTools.
- **Is the third line necessary in the SURFACE card, like you show in the wt.in?**
    - Not necessary any more.
- **Is NP the number of layers of layered materials?**
    - No, it's not. It's used for surface state calculations. It's called the number of principal layers. You can find more information in Sancho's paper. "Highly convergent schemes for the calculation of bulk and surface Green functions, M P Lopez Sancho, J M Lopez Sancho, J M L Sancho and J Rubio, J.Phys.F.Met.Phys.15(1985)851-858"
- **Will the selection of NumOccupied tag affect the anomalous Hall conductivity calculation?**
    - No. The AHC calculation doesn't depend on NumOccupied.
- **Is there any way to study double inversion? When we set NumOccupied we only study between bands NumOccupied and NumOccupied+1.**

    - I am not sure whether we can use WCC to study double inversion. If not, then we can't study it.
- **The "slab" is really a ribbon in this case, since the original system is 2D, right?**
    - Yes, if the original system is 2D, then "slab" means a ribbon. The surface states are called edge states.
- **Why Z2 number in the Chern insulator phase the gap goes to zero?**
    - The Z2 number is only defined in the system with time-reversal symmetry. So the Z2 value in the WT.out for time-reversal breaking system is meaningless.
- **What is the meaning of blue and red colors in the slabek.png plot?**
    - The color indicates the weight of projections onto surfaces. The blue (red) color is the weight on the top (bottom) surface.
- **What's the difference between the surfdos and surfdos_only files?**
    - The surfdos is for the surface state spectrum. surfdos_only is only used to make surface states more visible by removing the bulk spectrum. It's useful for QPI calculation. Usually, don't use this plot for publication.
- **Will this work for systems with defects, oxygen vacancies, etc.?**
    - If you treat it as a periodic system, then yes.
- **What is the blue line in the WCC plot?**
    - The blue line is an automatically generated line to get the Z2 number by counting how many crossing times between the blue line and the red WCC spectrum. Get more information on this paper (Soluyanov 2011 PRB). Please remove it when using it for publication.
- **Is it possible to get a tight-binding model just for the topological bands?**
    - No. It's not possible.
- **Bi2Se3 is not a cubic lattice, but we calculate the topological index in cubic planes? I don't understand?**
    - We need to get Z2 number for six time-reversal invariant planes. It doesn't depend on what kind of lattice.
- **For Bi2Se3 surface states, we need 5 quintuple layers. Is there minimum criteria for Nslab here to get surface states?**
    - No, the thickness depends on the material.
- **How do you chose the radius of the ball around the Weyl point? The chirality results should be radius dependent?**
    - You should decrease the radius until the Weyl chirality doesn't change which means that the sphere only encloses one Weyl point.
- **Why the chirality is only +-1? It should be the magnetic 'monopole' charge.**
    - Actually, the chirality could be +-2 or +-3 if there is some symmetry to protect the Weyl points.
- **Is there a big difference between NSLAB and Green's function surface states?**
    - They should be the same if Nslab is large enough. SlabBand_calc will give you surface states of both dual surfaces. While SlabSS_calc will give you surface state for the semi-infinite system.

- **Is it the chirality even under time-reversal? Should we find the same value for the chirality?**
    - Yes, the chirality is even under time reversal. That is why you have a minimum of four Weyl points in Weyl semimetals with time-reversal symmetry (and broken inversion). The total chirality in the BZ must vanish, but time reversal maps one Weyl point onto another of the same chirality. So you need two more with the opposite chirality.