

Report for the Wannier wave function calculation

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ABINIT is a software suite to calculate the optical, mechanical, vibrational, and other observable properties of materials based on the density function theory (DFT). In this report, we use the Wannier90 interface to compute the Maximally Localized Wannier Functions (MLWFs), and present detailed steps to calculate the Wannier functions and the electronic band structure of silicon.

I. THEORY AND ALGORITHM

In this report, we calculate the MLWFs and related property of silicon based on DFT method, as a practice of mapping DFT method to a tight-binding model. The traditional DFT calculation is deeply rooted in the nearly free electron perspective, where the calculation is in the momentum space. However, the Wannier function provides an alternative and also complimentary view points from the tight-binding approximation in the real space. By computing the MLWFs, one can obtain the knowledge about the localized wave functions around specific atoms, analyze the nature of chemical bonding, and also probe the phenomenon related to electric polarization and orbital magnetization. As an important application, Wannier interpolation can extend quantities computed on a coarse reciprocal-space mesh into much finer meshes at low cost.

Electronic structure calculation are often carried out using periodic boundary condition, and people use Bloch orbitals $\psi_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$ as common eigenstates, where $u_{n\mathbf{k}}$ has the same periodicity as the Hamiltonian. With the Fourier transformation of the momentum \mathbf{k} , one can construct the Wannier function

$$|\mathbf{R}n\rangle = \frac{V}{(2\pi)^3} \int_{BZ} d\mathbf{k} e^{-i\mathbf{k}\cdot\mathbf{R}} |\psi_{n\mathbf{k}}\rangle. \quad (1)$$

The Wannier function $|\mathbf{R}n\rangle$ form an orthonormal set. The former transformation constitutes a unitary transformation between Bloch state and Wannier state.

The gauge freedom exists in the definition of the Bloch state, where an additional phase $\psi_n(\mathbf{k})$ will not change the physical description of the system with $\psi_n(\mathbf{k})$ being any real function in reciprocal space. If the phase function is smooth, the Wannier wave function defined in Eq.1 will be well localized, due to the property of Fourier transformation that the smoother the reciprocal-space object, the more localized the resulting real-space object.

Things are more complicated in multiband case, where the gauge is generalized to any unitary transformation, compared with an additional phase $e^{i\psi_n(\mathbf{k})}$ in the single band case, i.e.

$$|\tilde{\psi}_{n\mathbf{k}}\rangle = \sum_{m=1}^J U_{mn}^{(\mathbf{k})} |\psi_{m\mathbf{k}}\rangle. \quad (2)$$

As mentioned above, the Bloch functions with different gauge yield Wannier function with different localization property. Note that the localized Wannier function can be used to perform downfolding of the band structure onto a minimal basis, which has remarkable benefits in numerical calculation. Therefore, people are motivated to search for the maximally localized wave functions (MLWFs).

Here, we define the localization functional as

$$\Omega = \sum_n [\langle 0n | r^2 | 0n \rangle - \langle 0n | \mathbf{r} | 0n \rangle^2] = \sum_n [\langle r^2 \rangle_n - \bar{\mathbf{r}}_n^2] \quad (3)$$

to measure the sum of the quadratic spreads of the wave functions in the home unit cell around their centers. Then, we can express Ω in terms of the Bloch wave functions. Once a \mathbf{k} -space expression for Ω has been derived, MLWFs can be obtained by minimizing it with respect the $U_{mn}^{\mathbf{k}}$. This is done as a postprocessing step after a conventional electronic structure calculate has been self-consistently converged and a set of ground state Block orbitals $|\psi_{m\mathbf{k}}\rangle$ has been chosen. In this manner, one can compute the MLWFs in real space.

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The MLWFs can be used to perform Wannier interpolation, where the wave functions can be used as an exact or very accurate tight-binding basis, allowing one to perform a number of operations on top of a conventional first-principles calculation very efficiently and accurately.

The actual first-principles calculation is carried out on a relatively coarse grained uniform reciprocal-space mesh \mathbf{k} , where the quantity of interest $f(\mathbf{q})$ is calculated from the Bloch eigenstates. The states in the selected bands are then transformed into Wannier wave functions, and $f(\mathbf{q})$ is transformed accordingly into $F(\mathbf{R})$ in the Wannier representation. By virtue of the spatial localization of the Wannier wave function, $F(\mathbf{R})$ decays rapidly with $|\mathbf{R}|$. Starting from this short-range real-space representation, the quantity f can now be accurately interpolated onto an arbitrary point \mathbf{k} in reciprocal space by carrying out an inverse transformation.

One can use Wannier interpolation to generate band structure plots. From the Wannier functions spanning a group of J bands, we can Fourier transform the MLWFs, i.e.,

$$|\psi_{n\mathbf{k}}^W\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} |\mathbf{R}n\rangle. \quad (4)$$

Here, the states $|\psi_{n\mathbf{k}}^W\rangle$ are not eigenstates of the Hamiltonian, and we say they belong to the Wannier gauge.

At given \mathbf{k} , the Hamiltonian matrix elements is represented in the Wannier gauge by

$$H_{\mathbf{k},nm}^W = \langle \psi_{n\mathbf{k}}^W | H | \psi_{m\mathbf{k}}^W \rangle = \sum_{\mathbf{R}} \langle \mathbf{0}n | H | \mathbf{R}m \rangle. \quad (5)$$

In general this is a nondiagonal matrix in the bandlike indices, and the interpolated eigenenergies are obtained by diagonalization,

$$H_{\mathbf{k},nm}^H = [U_{\mathbf{k}}^\dagger H_{\mathbf{k}}^W U_{\mathbf{k}}]_{nm} = \delta_{nm} \epsilon_{n\mathbf{k}}. \quad (6)$$

Note that the momentum \mathbf{k} is chosen arbitrarily, therefore, we can calculate the eigenenergies of all \mathbf{k} points in the reciprocal space. Here, the cost of calculation corresponds to J , the number of Wannier functions per cell, which is typically much smaller than the number of basis function, say plane waves given a cutoff value, used in the traditional DFT method. Therefore, the Wannier interpolation provides an efficient method to plot the electronic band structure.

II. NUMERICAL CALCULATION

Wannier90 is a code that computes MLWFs. To obtain the MLWFs, the code minimize the spread of the wave function with respect to the choice of phase, which is done by using a steepest-descent algorithm. After the self-consistent ground state calculation performed, ABINIT code computes the overlap $M_{mn} = \langle u_{m\mathbf{k}} | u_{n\mathbf{k}+\mathbf{b}} \rangle$ between the cell periodic part of the Bloch states $|u_{k\mathbf{n}}\rangle$, and sends the value to Wannier90. Then, Wannier90 will start the minimization process based on the guessing projection $A_{mn} = \langle u_{m\mathbf{k}} | g_n \rangle$ of the Bloch state $|g_n\rangle$ onto trial localized orbitals $|g_n\rangle$. In this tutorial, Wannier90 is included as a library in ABINIT and the calculation is automatics, so that in a single run we can do both the ground state calculation and the computation of MLWFs.

However, we mention that Wannier90 can run with other computation software, like VASP, FLEUR, OPENMX and Quantum ESPRESSO. In the original tutorial of Wannier90, the code is run with the PWSCF interface of quantum ESPRESSO. I struggled to run the example in the chapter 18 Iron - Berry curvature, anomalous Hall conductivity and optical conductivity, but failed. In these attempts, I downloaded the Wannier90 package independently, and installed related quantum ESPRESSO software. Wannier90 worked fine for the first several samples in the tutorial, but reported a computational error in the example in chapter 18. It seems to be a common problem of this specific tutorial sample, and some people post this problem on the Internet. However, there is not a well-accepted, at least easily accessible, solution to this problem for now. I tend to believe that the problem is not from the Wannier90 code itself, but due to the improper input of the calculation. The input files for example 18 may need updating. By the way, PWSCF took a long time to finish the calculation, say typically 30 minutes for every single command because I compiled the quantum ESPRESSO in a serial version, and the performance can be enhanced in a parallel compiled version.

Let get back to the tutorial of Wannier90 in ABINIT. We conduct the computation of the MLWFs of silicon crystal as the first trial, and extract the Wannier functions corresponds to the four valence states of silicon.

Similar to the former tutorial, there are two steps to calculate the MLWFs. First, we perform the tradition ABINIT self-consistent calculation to generate the data in the reciprocal space, and then perform a non self-consistent calculation which call the Wannier90 library. The file wannier90.win is mandatory as the input of Wannier90. In such file, we specify the number of Wannier functions to extract, and the maximum number of iterations.

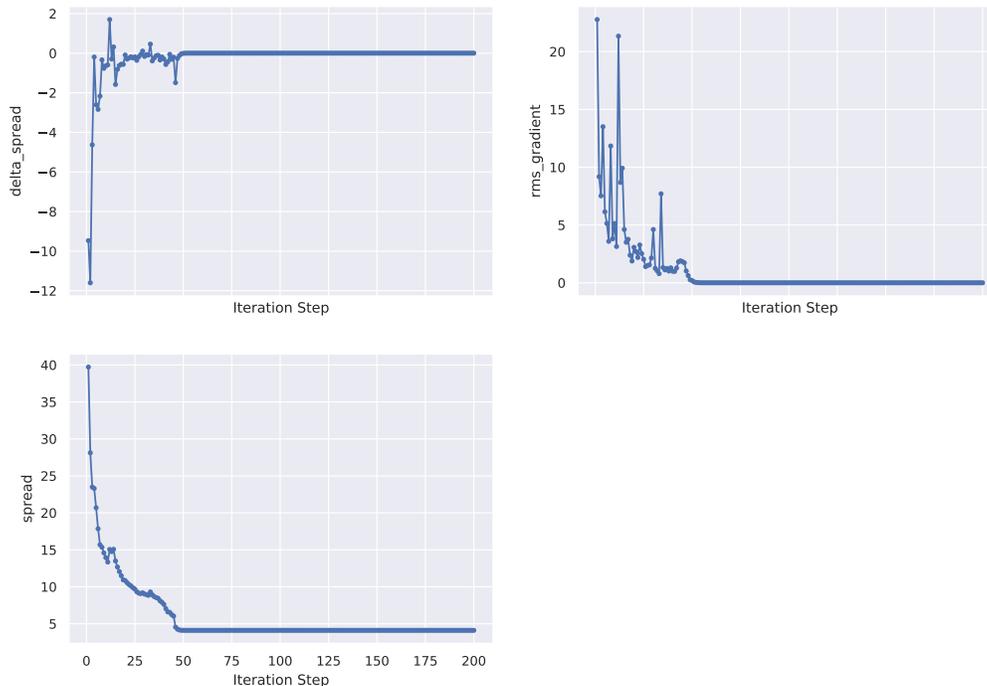


FIG. 1. The spread of Wannier wave functions in the iterations.

In the Fig.2 and Fig.2, we can see that the Wannier functions reach the convergence after 50 iteration steps, where the center of Wannier functions keep stable, and the spread of the function is minimized. Then, after the calculation, the MLWFs is documented in the wannier90_0000x.xsf file, where x is from 1 to 4, corresponding to four MLWFs of silicon atoms. We can use the Xcrysden software to visualize the Wannier functions, as shown in Fig.3. From the figure, the four Wannier functions orientates in four degenerate directions, which corresponds to the four equivalent sp^3 hybridization orbitals.

Having obtained the MLWFs of silicon atoms, we can use the Wannier functions to calculate the band structure in a different way from the traditional DFT. In this part, we first perform a self-consistent run to get the electron density of the silicon crystal which include 5 bands. Then, we perform a non self-consistent run, and expand the number of bands to 14. At the final run, we call the Wannier90 library and calculate the MLWFs according to the calculation output of the first two runs. After obtaining the MLWFs of silicon atoms, we run Wannier90 in standalone mode and compute the band structure. The output file is tw90_4o_DS3_w90_band.gnu, which can be visualize by gnuplot package easily, as shown in Fig.4 .

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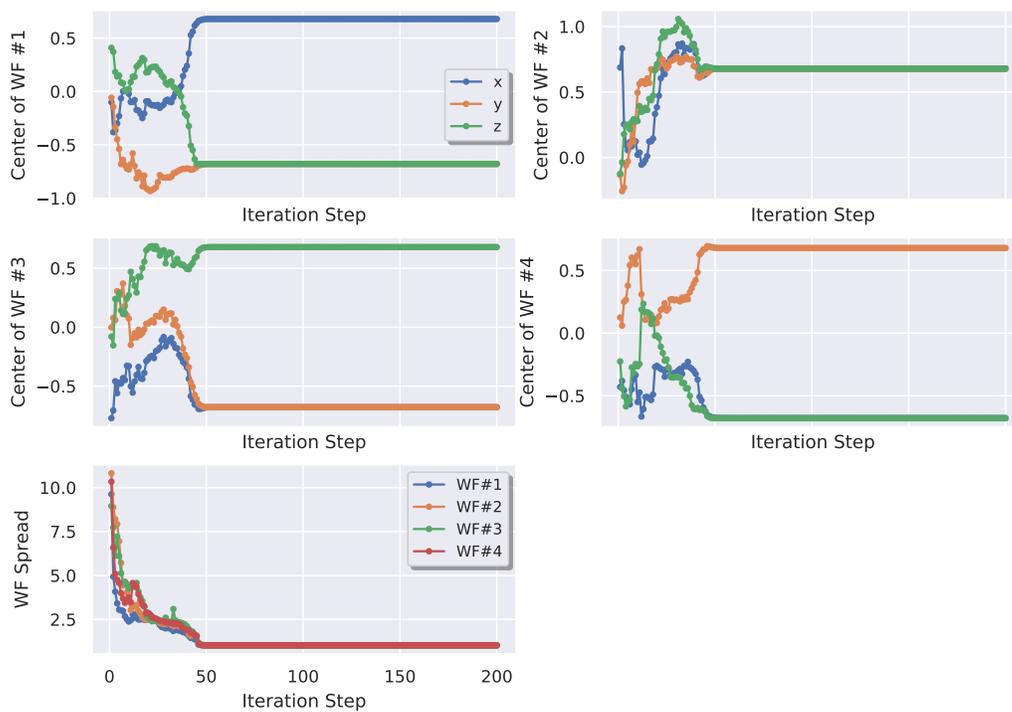


FIG. 2. Convergence of parameters in the iterations.

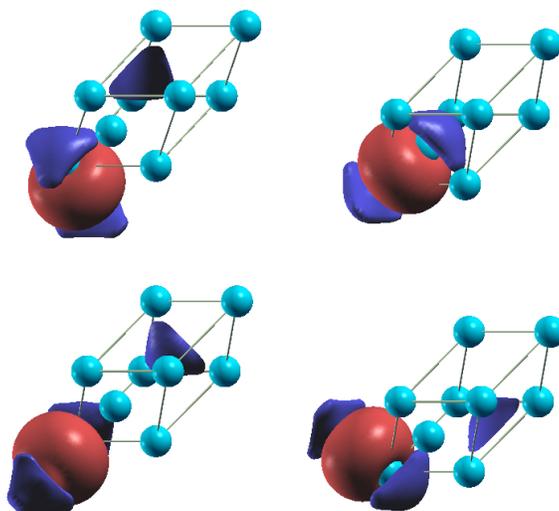


FIG. 3. The four MLWFs of silicon atoms in different orientations.

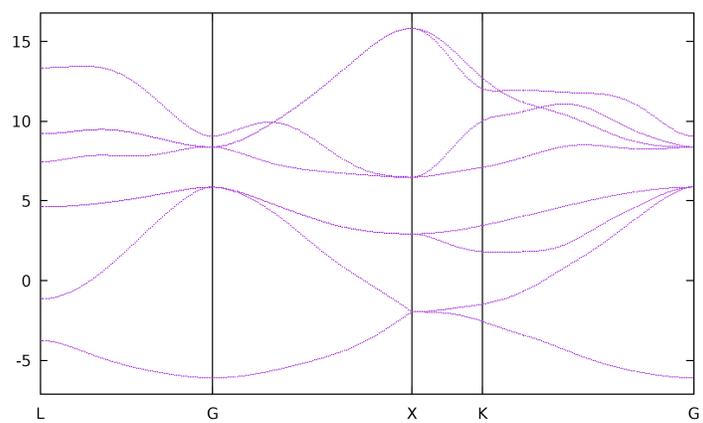


FIG. 4. The band structure of silicon atoms.