

Procedure:

1. Click the exe file. Afterward, the Image1 will appear. Wait for about one minute until the Image2 appears, and then you can start using the software.

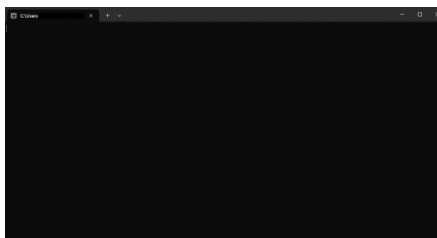


Figure 1

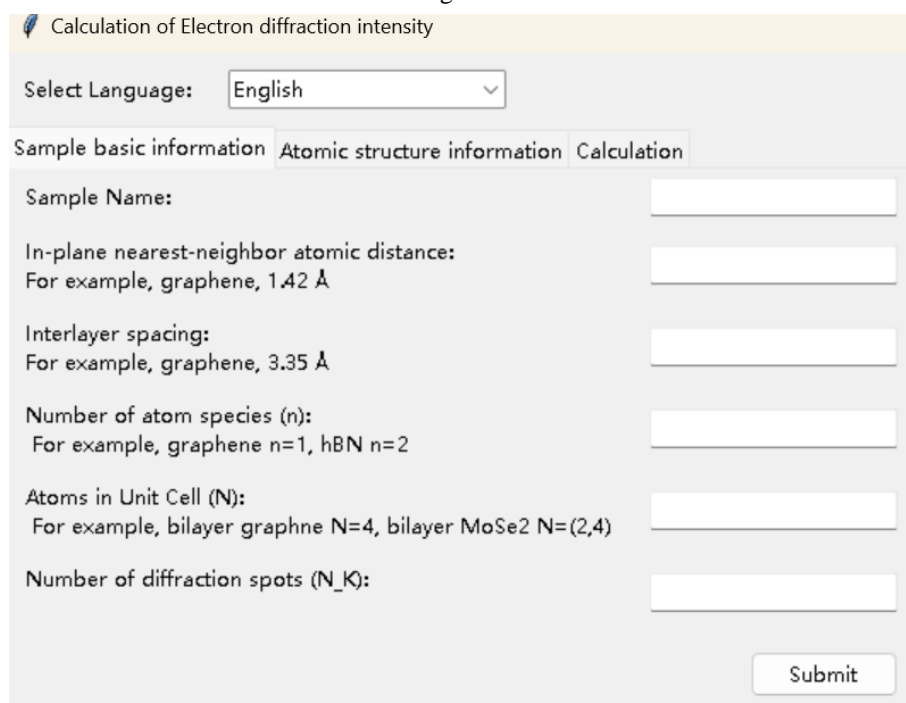


Figure 2

2. Selection Language: offers two options, English and Simplified Chinese.
3. Page 1 (Sample Basic Information). You need to enter the sample name, in-plane nearest-neighbor atomic distance, interlayer spacing, number of layers, number of atoms in the unit cell, and the number of diffraction spots to be calculated. Except for the sample name, the other inputs should be numeric values (positive numbers). Click the 'Submit' button at the bottom after filling in the information.
4. Page 2 (Atomic Structure Information). You could click the “Back” button to return to the previous page. You need to enter the atomic coordinates in the unit cell, diffraction point coordinates, f-values, and tilt axis information (including the number of tilt points, the range of tilt, and the tilt axis). You could click the “More Info” to check the literature “Relativistic Hartree-Fock X-ray and electron scattering factors” and calculate the f-values. Click the 'Submit' button at the bottom after filling in the information.
5. Page 3 (Calculation). Here, you can click the 'Back' button to return to the previous page.

Click 'Show Information' to check if the information entered on the previous two pages matches your expectations. If not, go back and make corrections. You can also save or import information here. Click the 'Calculate' button to view the results (image). Below, you can directly save the images (png, jpg) or save the calculation data (txt, xlsx, csv).

Example1 (bilayer graphene):

1. Input basic information

Calculation of Electron diffraction intensity

Select Language: English

Sample basic information Atomic structure information Calculation

Sample Name: Bilayer graphene

In-plane nearest-neighbor atomic distance:
For example, graphene, 1.42 Å 1.42

Interlayer spacing:
For example, graphene, 3.35 Å 3.35

Number of atom species (n):
For example, graphene n=1, hBN n=2 1

Atoms in Unit Cell (N):
For example, bilayer graphene N=4, bilayer MoSe2 N=(2,4) 4

Number of diffraction spots (N_K): 3

Submit

2. Input atomic structure information. (There is a scrollbar on the right. Ensure that each piece of information is filled in correctly and click 'Submit')

Calculation of Electron diffraction intensity

Select Language: English

Sample basic information Atomic structure information Calculation

Back

Atom Coordinates (x, y, z):
Input the coefficient coordinates. For example, (a,2a,c) should be entered as (1,2,1)

0	0	0
1.732 $\sqrt{3}$	1	0
0.866 $\sqrt{3}/2$	0.5	1
1.732	1	1

Diffraction Coordinates (x, y, z):
Input coefficient coordinates. For example, (1/a, 3/a, 1/d) should be entered as (1,3,1)

-0.577 $-\sqrt{3}/3$	0.333 $1/3$	0
0	0.667	0
-0.577	1	0

f Values:
Click the More Info button to check the literature and calculate the f value by yourself

More Info

1.256

1.256

0.591

Rotation Axis Info:

Number of tilt points:

200 Don't too little

Tilt range (the starting point and endpoint of the tilt):

-15 15

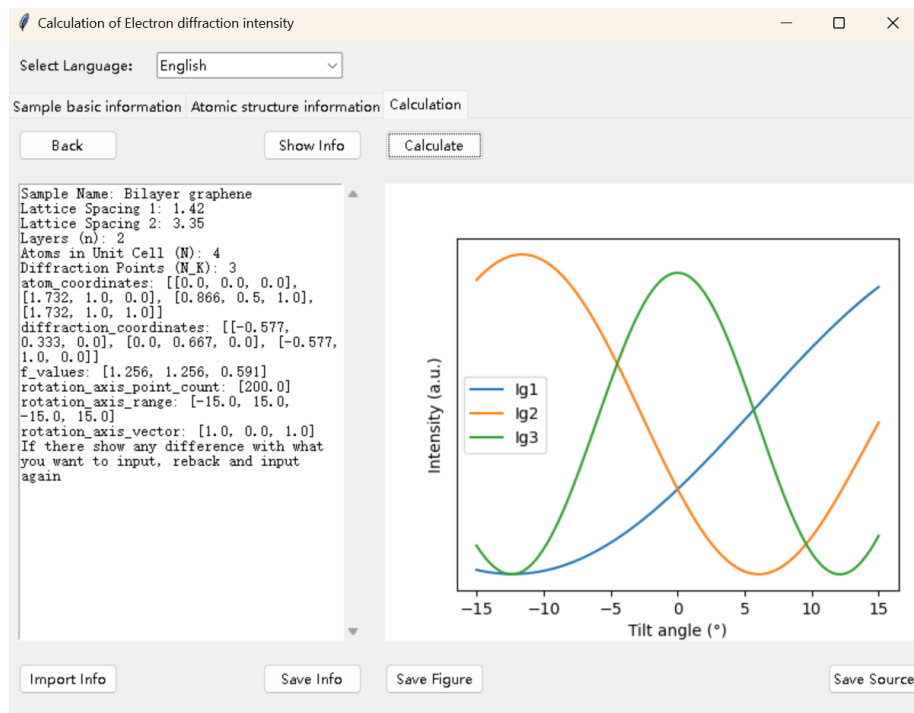
Rotation Axis Vector (Rx, Rz, Signaly):
Rx and Rz are the components of the tilt axis in the x and z directions, respectively. Signaly takes a non-zero value

1 0 1

$R_x^2 + R_z^2 < 1, R_y^2 = 1 - (R_x^2 + R_z^2)$

Submit

- Calculate. Here, I have also provided a file for bilayer graphene that can be used directly for calculations. You can import it and perform the calculations.



After saving the crystal information (.json), you can modify the corresponding information on the second page using a Python editor (such as Visual Studio Code or Jupyter notebook), then import it for calculation (of course, ensure that the information entered is correct).

Example2 (AA'-stacked MoSe₂)

1. Input basic information. **Note that here n=2, the following N input n values (comma apart), each is the number of n kinds of atoms in the unit cell.**

Calculation of Electron diffraction intensity

Select Language: English

Sample basic information | Atomic structure information | Calculation

Sample Name: AA'-stacked MoSe2

In-plane nearest-neighbor atomic distance:
For example, graphene, 1.42 Å: 2.04

Interlayer spacing:
For example, graphene, 3.35 Å: 13

Number of atom species (n):
For example, graphene n=1, hBN n=2: 2

Atoms in Unit Cell (N):
For example, bilayer graphene N=4, bilayer MoSe2 N=(2,4): 2,4

Number of diffraction spots (N_K): 3

Submit

2. Input atomic structure information. (There is a scrollbar on the right. Ensure that each piece of information is filled in correctly and click 'Submit'). **The atomic coordinates and f values should be entered in the order of the n kinds of elements on the first page.**

Calculation of Electron diffraction intensity

Select Language: English

Sample basic information Atomic structure information Calculation

Back

Atom Coordinates (x, y, z):
Input the coefficient coordinates. For example, (a,2a,c) should be entered as (1,2,1)

0.866	0.5	0.25	Mo atoms
0	0	0.75	
0	0	0.13105	Se atoms
0	0	0.36895	
0	1	0.63105	
0	1	0.86895	

Diffraction Coordinates (x, y, z):
Input coefficient coordinates. For example, (1/a, 3/a, 1/d) should be entered as (1,3,1)

-0.557	0.333	0
0	0.667	0
-0.557	1	0

f Values:
Click the More Info button to check the literature and calculate the f value by yourself

5.875	f_Mo N_K=1,2,3
5.875	
3.622	
4.6715	f_Se N_K=1,2,3
4.6715	
2.849	

More Info

Rotation Axis Info:

Number of tilt points:
200

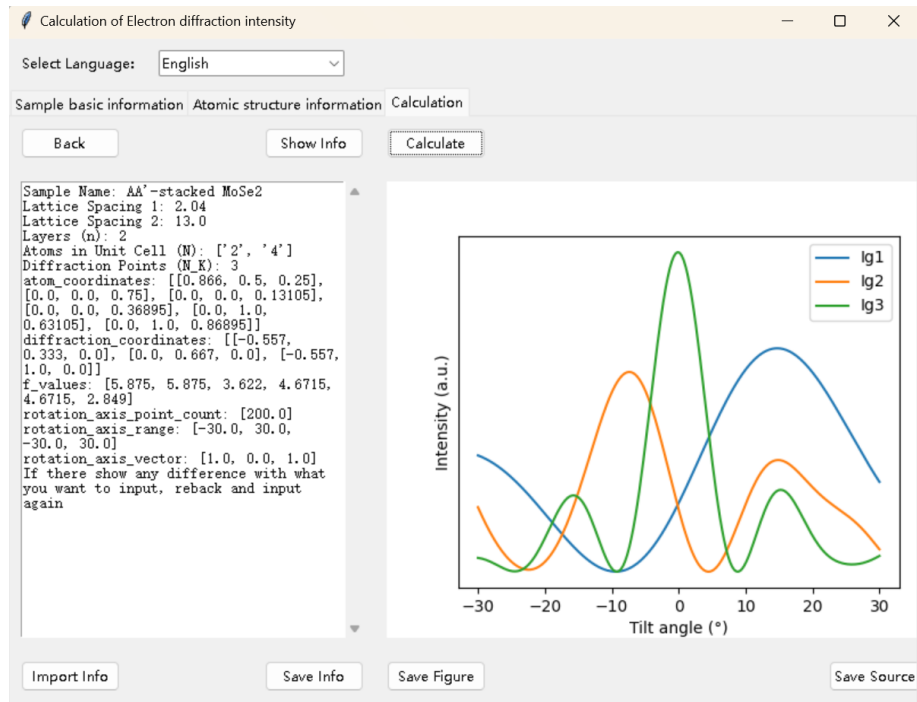
Tilt range (the starting point and endpoint of the tilt):
-30 30

Rotation Axis Vector (Rx, Rz, Signaly):
Rx and Rz are the components of the tilt axis in the x and z directions, respectively. Signaly takes a non-zero value

1	0	1
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Submit

- Calculate. A file of bilayer AA'-stacked MoSe₂ is provided, and you can import it and perform the calculation.



Calculation of f values:

Taking graphene as an example, $s=K/2$ in the table (from the literature of “More Info” in Page2), where K is the length of the diffraction spot. For instance, for $(-\sqrt{3}/3x, 1/3x, 0d)$, s is approximately 0.235. The table contains s values of 0.20 and 0.25. Assuming that $f(s)$ varies linearly between the two given s values, we get $f=1.256$.

P. A. DOYLE AND P. S. TURNER

Table 2. *Kinematic electron scattering factors**

* These values must be multiplied by $m/m_0=(1-v^2/c^2)^{-1/2}$ for electrons of velocity v .

S	2 HE	3 LI	4 SE	5 B	6 C	7 N	8 O	9 F	10 NE	11 NA	12 MG
0.00	0.418	3.286	3.052	2.794	2.509	2.211	1.983	1.801	1.652	4.778	5.207
0.05	0.410	2.830	2.907	2.638	2.406	2.144	1.937	1.767	1.626	4.138	4.717
0.10	0.390	1.879	2.237	2.250	2.138	1.963	1.808	1.671	1.552	2.967	3.656
0.15	0.359	1.166	1.635	1.791	1.795	1.718	1.625	1.532	1.443	2.099	2.657
0.20	0.323	0.753	1.151	1.377	1.460	1.458	1.422	1.371	1.313	1.594	1.953
0.25	0.286	0.526	0.832	1.048	1.168	1.216	1.222	1.206	1.176	1.295	1.502
0.30	0.250	0.396	0.614	0.803	0.932	1.006	1.040	1.049	1.043	1.095	1.211
0.35	0.217	0.314	0.469	0.625	0.748	0.831	0.881	0.908	0.918	0.946	1.013
0.40	0.189	0.259	0.371	0.497	0.606	0.689	0.747	0.784	0.805	0.827	0.868