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.

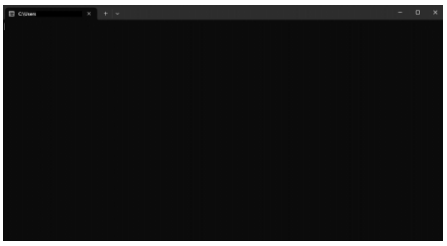


Figure 1

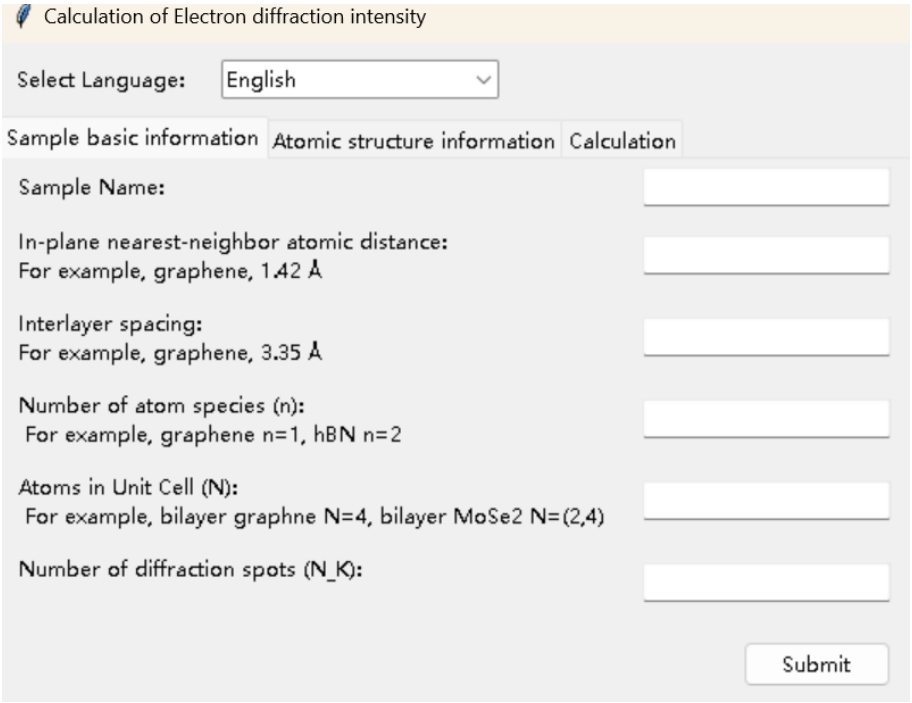


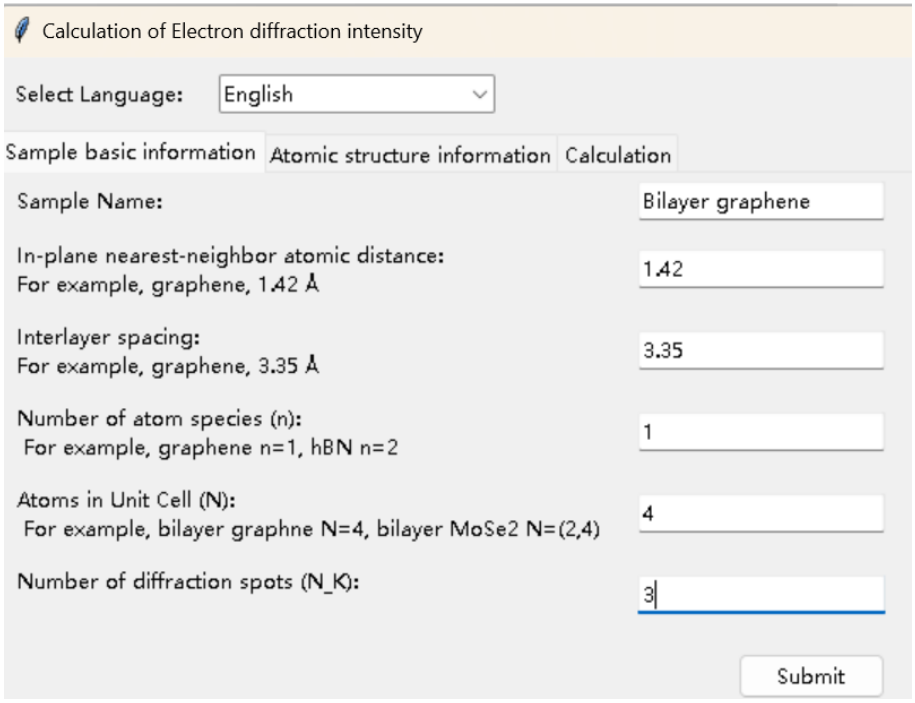
Figure 2

2. Selectioin 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.

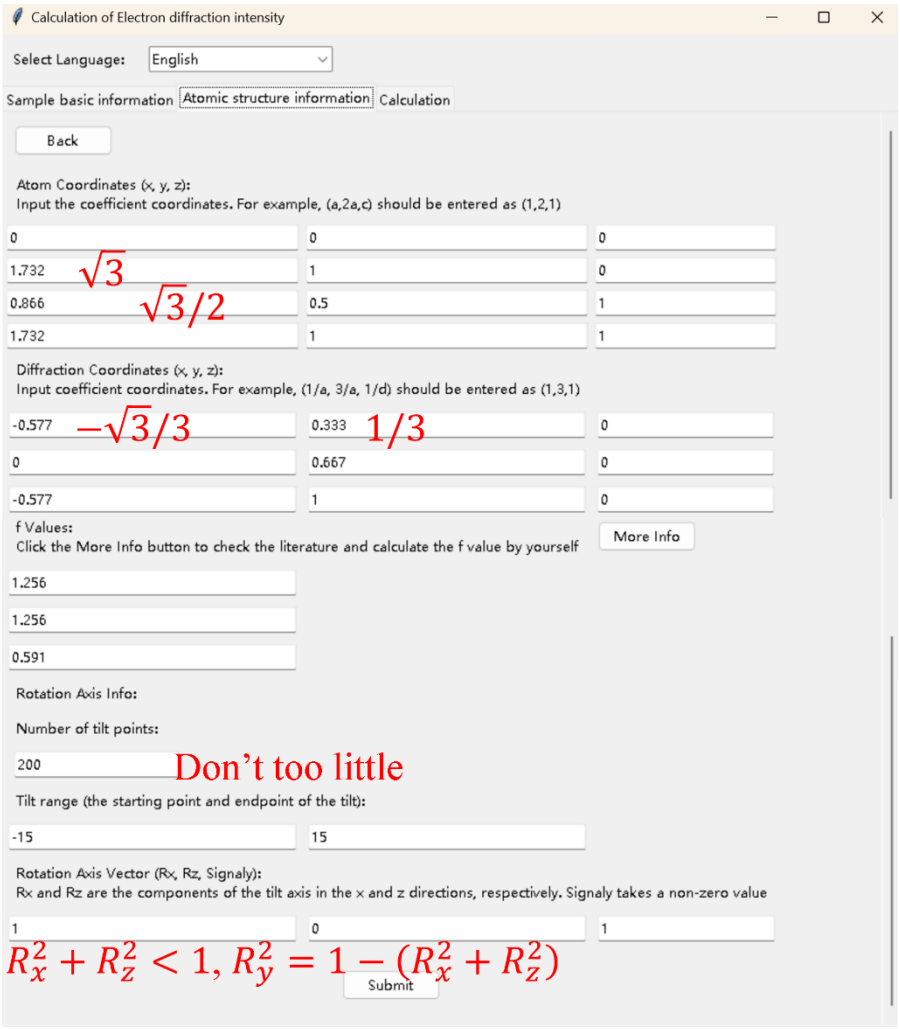
Click 'Show Information' to check if the information entered on the previous two pages matches your expectations. If not, go back and make corrections. You can also save or import information here. Click the 'Calculate' button to view the results (image). Below, you can directly save the images (png,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

Example1 (bilayer graphene):

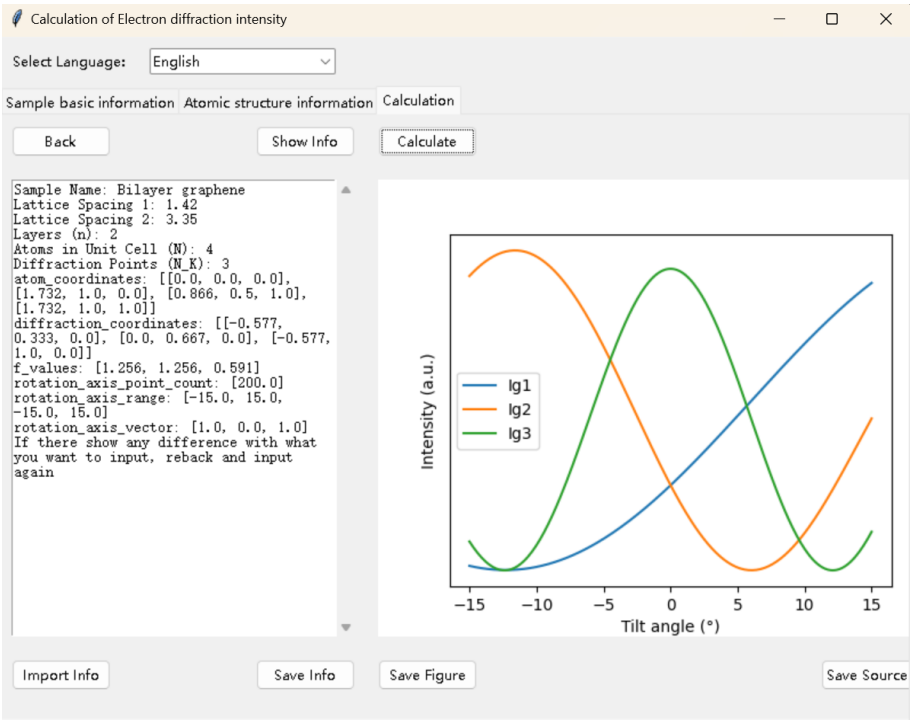
1. Input basic information



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')



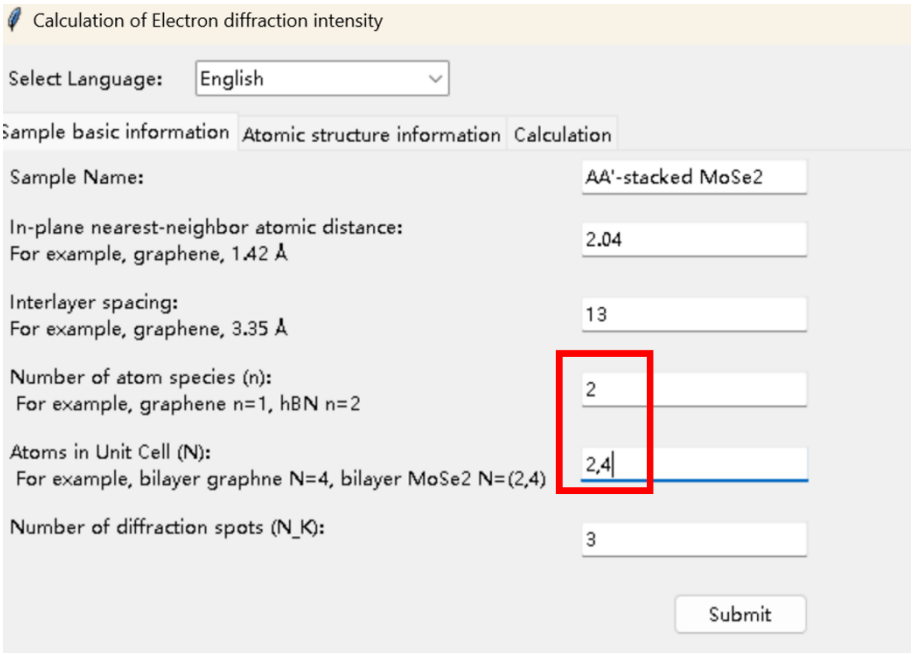
3. Calculate. Here, I have also provided a file for bilayer graphene that can be used directly for calculations. You can import it and perform the calculations.



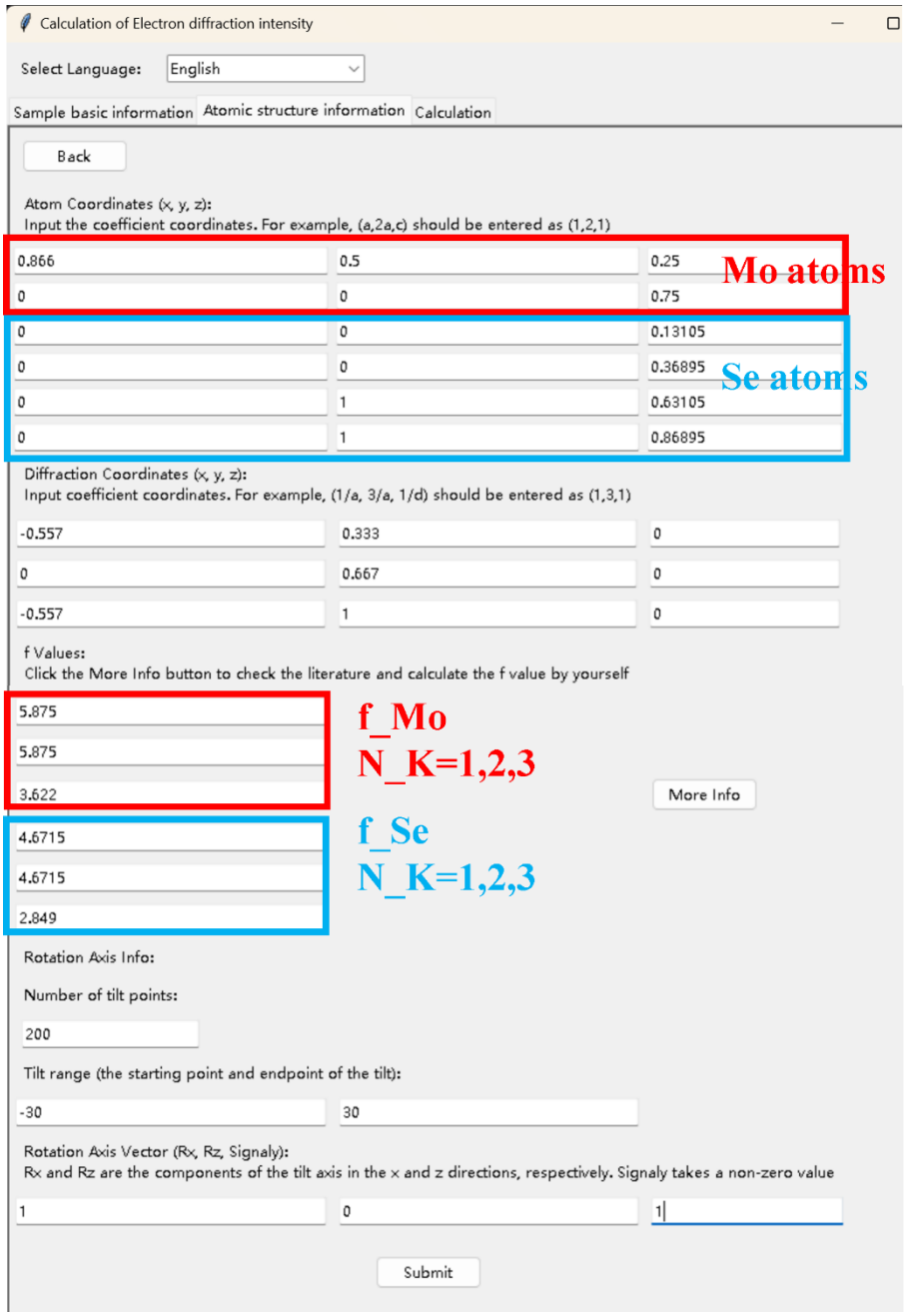
After saving the crystal information (.json), you can modify the corresponding information on the second page using a Python editor (such as Visual Studio Code or Jupyter notebook), then import it for calculation (of course, ensure that the information entered is correct).

Example2 (AA'-stacked $MoSe_2$)

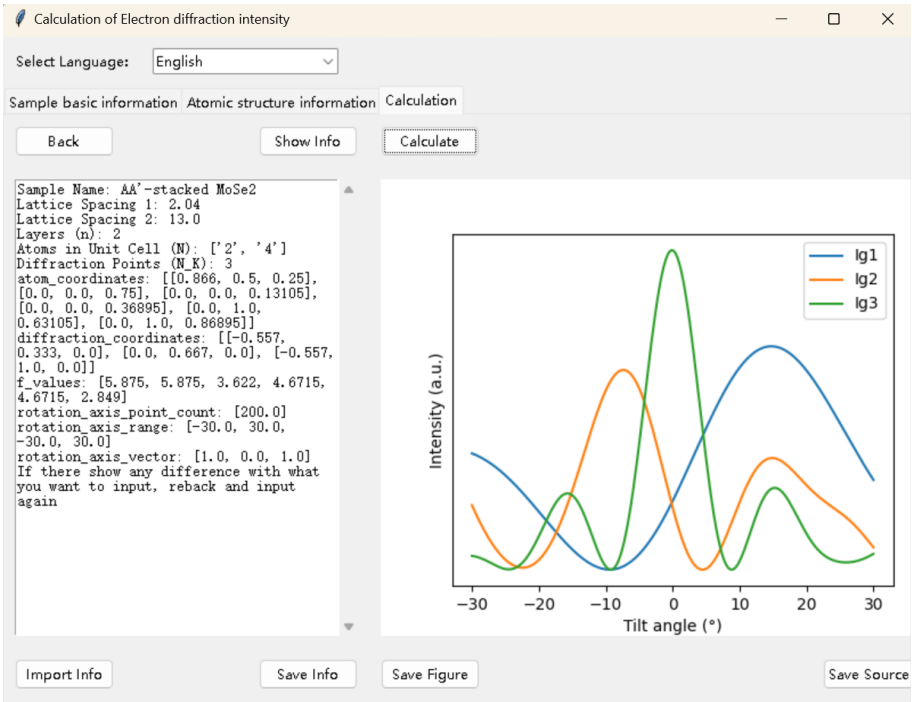
1. Input basic information. **Note that here n=2, the following N input n values (comma apart), each is the number of n kinds of atoms in the unit cell**.



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**.



3. 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 $\left(-\sqrt{3}/3x\,,1/3x\,,0d\right)$, 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.

	2	3	4	5	6	7	8	9	10	11	12
S	HE	LI	BE	B	C	N	O	F	NE	NA	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	2.807	2.638	2.405	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	1.161	1.377	1.469	1.458	1.422	1.371	1.313	1.594	1.953
0.25	0.286	0.526	0.837	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