Lecture "Advanced Material Modeling"
Skolkovo Institute of Science and Technology
"Advanced materials properties" lab (lab #1)
Complement of information : vizualisation

A. Foreword

Vizualisation of data for first-principles software applications (FP apps) relies on different software technologies than the FP code themselves. Hence, many third-party vizualisation (VIZ) tools exist, not directly linked with the FP code developer team. Some VIZ tools will actually work with different FP codes, and the data for some FP code can be vizualized with different VIZ tools.

These VIZ tools might be suitable for some platform, but not all. As an example, vizualisation most often cannot done on the high-performance computer used to run FP apps. Also, it might be that the compatibility between a FP code and a VIZ tool is broken when new versions are issued, due to format changes.

In the present context of COVID-19, no standard solution exists, as vizualisation is likely to be done on the personal computer. The present document might be improved in the coming days.

B. Abipy and scripts inside the ABINIT package.

ABINIT has its own library of python script for vizualisation, called Abipy.
See https://docs.abinit.org/topics/Abipy . A galery of plots is available at
http://abinit.github.io/abipy/gallery/index.html .
Installation of the prerequisite of Abipy needs some human time and skill. It is described at length
in github.com/abinit/abipy (scroll this page until you reach the "Getting Abipy" section). It is by far the preferred vizualisation tool for ABINIT, but the installation might prevent you to use it.

Some other tools to draw plots (e.g. band structures) are available inside the ABINIT package, see the directory scripts/post_processing, with README file description of the content of the directory.

C. ABINIT interfaces to standard formatted data, that can be vizualised

To produce a CIF file, see "prtcif" docs.abinit.org/variables/dev/#prtcif
To produce a POSCAR file, see "prtposcar" docs.abinit.org/variables/dev/#prtposcar
ABINIT can read a POSCAR file, see "structure" docs.abinit.org/variables/basic/#structure
ABINIT can read a XYZ file, see "xyzfile" docs.abinit.org/variables/geo/#xyzfile

Thanks to its post-processor Cut3d docs.abinit.org/guide/cut3d/ ,
ABINIT can generate 3D density files in the .xsf format (XCrystDEN, VESTA)

D. Non-exhaustive list of VIZ tools for ABINIT

(1) C2X   https://www.c2x.org.uk/
Version 2.34b released, 9th April 2020. Adds support for Abinit 9.0, and tries to avoid re-ordering species when writing Vasp or Abinit input files.

(2) VESTA http://jp-minerals.org/vesta
VESTA can vizualize the CIF, POSCAR and .xsf formats.

(3) XCRYSDEN http://www.xcrysden.org/ , works with the .xsf format .

(4) JMOL/JSMOL http://wiki.jmol.org/ , works with the .CIF format .