Development of the OpenMX Viewer

- What is the OpenMX Viewer?
- Codes of the OpenMX Viewer
- New functionalities
- Prospects

http://www.openmx-square.org/viewer/

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What is the OpenMX Viewer?

The OpenMX Viewer (Open source package for Material eXplorer Viewer) is a web-based graphical user interface (GUI) program for visualization and analysis of crystalline and molecular structures and 3D grid data in the Gaussian cube format such as electron density and molecular orbitals. The tool might be useful for educational purpose and getting started with the calculations for beginners.

Functionalities:

- Visualization of .dat, .xyz, .cif, .md, .cube, .Band files

- Animated visualization of the .md file

- Analysis of the structure and charge state

- Visualization of the 1st Brillouin zone

- Generation of the OpenMX input file

WEB-based GUI

- WEB browser is one of the most familiar interfaces that people spend a long time.

- Any machine dependent problems such as OS and version can be absorbed by WEB browsers in principle, which results in that a single frame will work for many different platforms like Windows, Mac, and Linux.

- No downloading and no plugging-in and no updating are required for users.

- Developers only have to change and modify codes on the server, by which all the users can get benefit.

- Many tools have been developed so that WEB-based GUI is fast and easy to use.

Continuous development of the OpenMX Viewer

OpenMX Viewer:

|	
Ver. 1.00: Aug. 19, 2016	Ver. 1.29: Feb. 16, 2020
Ver. 1.01: Aug. 20, 2016	Ver. 1.30: Apr. 12, 2021
Ver. 1.02: Aug. 30, 2016	Ver. 1.31: Jun. 18, 2022
Ver. 1.05: Sep. 17, 2016	Ver. 1.36: Jul. 06, 2022
Ver. 1.06: Oct. 21, 2016	Ver. 1.37: Jul. 10, 2022
Ver. 1.07: Dec. 13, 2016	Ver. 1.38: Jul. 12, 2022
Ver. 1.08: Dec. 27, 2016	Ver. 1.39: Jul. 16, 2022
Ver. 1.09: Mar. 08, 2017	Ver. 1.40: Aug. 03, 2022
Ver. 1.10: Apr. 08, 2017	Ver. 1.41: Aug. 07, 2022
Ver. 1.11: Apr. 29, 2017	Ver. 1.42: Aug. 08, 2022
Ver. 1.12: May 05, 2017	Ver. 1.43: Aug. 08, 2022
Ver. 1.13: Dec. 08, 2017	Ver. 1.44: Aug. 09, 2022
Ver. 1.14: Dec. 25, 2017	Ver. 1.45: Aug. 09, 2022
Ver. 1.15: Dec. 25, 2017	Ver. 1.46: Aug. 09, 2022
Ver. 1.16: Jan. 31, 2018	Ver. 1.47: Aug. 12, 2022
Ver. 1.17: Feb. 06, 2018	Ver. 1.48: Sep. 20, 2022
Ver. 1.18: Feb. 23, 2018	Ver. 1.49: Nov. 11, 2022
Ver. 1.19: Feb. 24, 2018	Ver. 1.52: Feb. 01, 2023
Ver. 1.20: Feb. 25, 2018	Ver. 1.53: Feb. 01, 2023
Ver. 1.21: Feb. 25, 2018	Ver. 1.54: Feb. 10, 2023
Ver. 1.22: Mar. 01, 2018	Ver. 1.55: Feb. 15, 2023
Ver. 1.23: Mar. 05, 2018	Ver. 1.56: Jul. 15, 2023
Ver. 1.24: Mar. 23, 2018	Ver. 1.57: Jul. 17, 2023
Ver. 1.25: Sep. 09, 2019	
Ver. 1.26: Nov. 14, 2019	
Ver. 1.27: Nov. 14, 2019	
Ver. 1.28: Jan. 03, 2020	

Manual:

1st edition: Jul. 17, 2022
2nd edition: Feb. 02, 2023
3rd edition: Jul. 27, 2023

Without downloading and installing update versions, users can always access the latest version by just visiting the website.

Actual use per month of the OpenMX Viewer

Every day, the OpenMX Viewer is utilized for the actual use about 100 times.
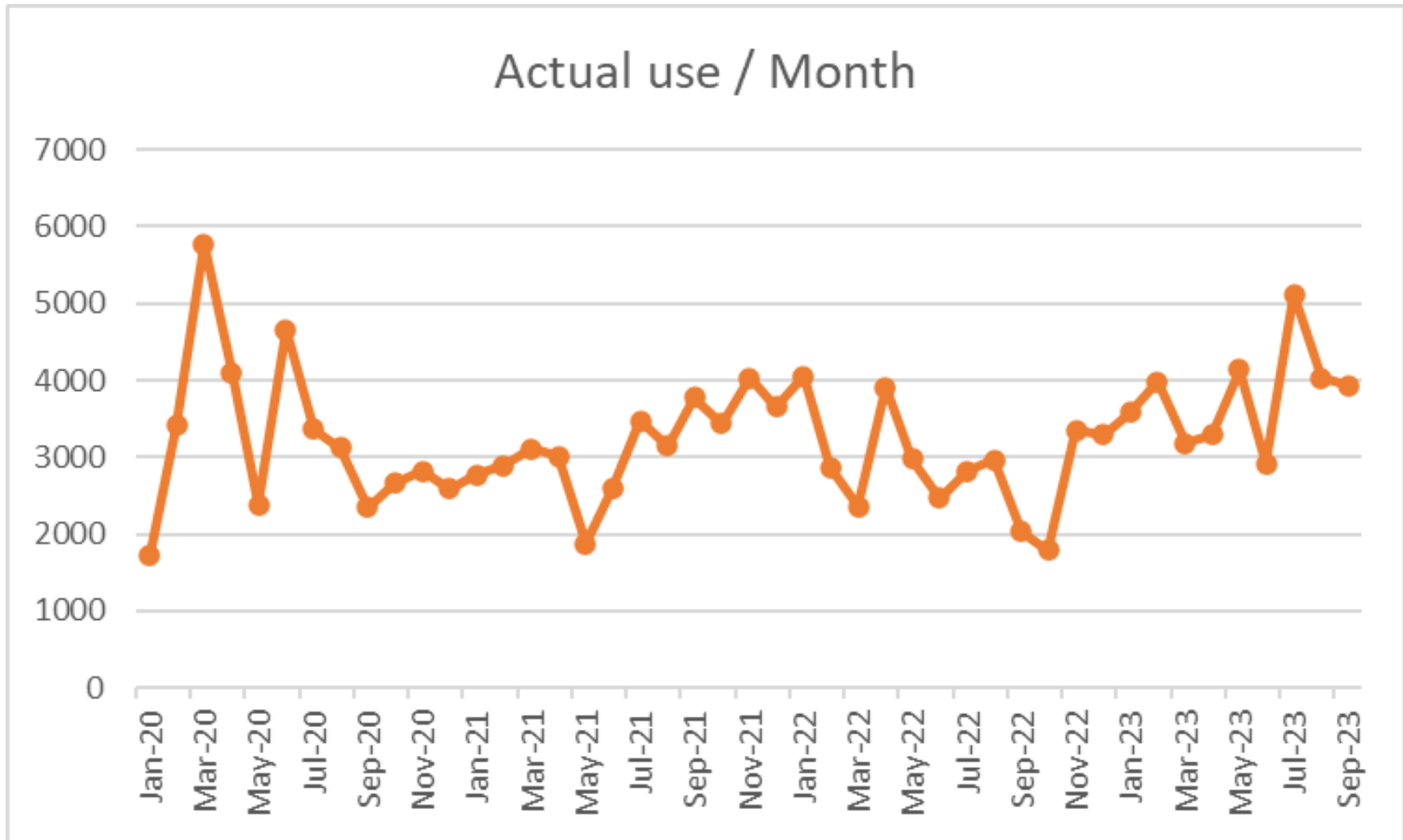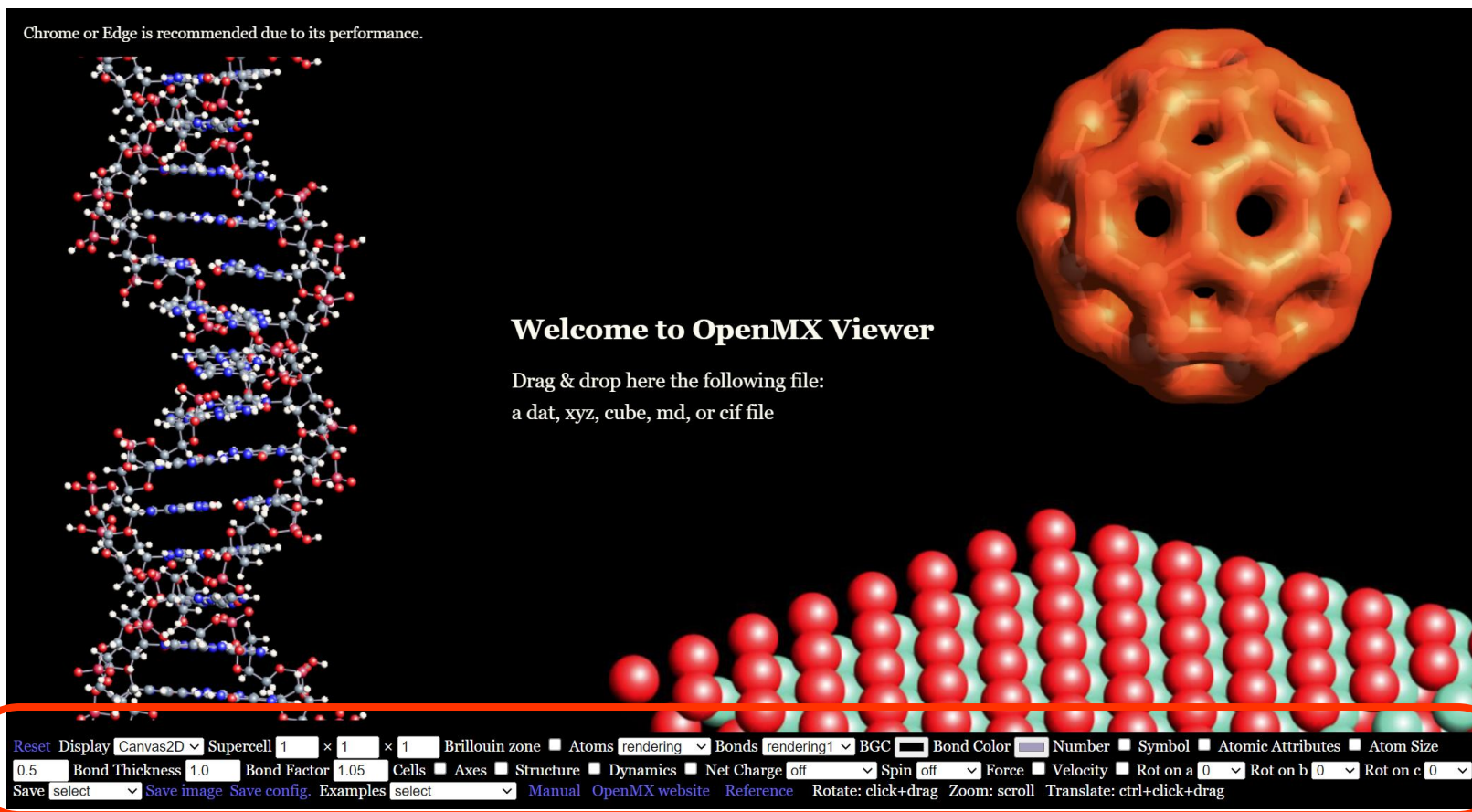
Codes of the OpenMX Viewer

The codes have been developed using HTML5, CSS3, javascript, Canvas2D, WebGL, CGI, and several javascript libraries as listed below:

Main code: index.html (7555 lines)
css file: style-viewst.css
WebGL libraries: three.min.js, THREEx.FullScreen.js,
                      THREEx.screenshot.js, BufferGeometryUtils.js
cif analysis: cif.js
Control panel: dat.gui.min.js, cnp.jp
Brillouin zone: brillouin.js
Input file analysis: analysis_inputfiles.js
cube file analysis: is_cube.js, is_nccube.js, marchingcubes.js,
                      marchingtetrahedra.js, surfacenets.js
Generation of input files: save_files.js

The total number of lines of codes is 33266 as of Nov., 2023.

Getting started with the OpenMX Viewer

Visit the website: http://www.openmx-square.org/viewer/
and drag & drop a dat, xyz, cube, md, or cif file on the site.
Then, you will see the structure of your model.

Here is the main control panel as we will explain in the next slides.

Examples

■ Examples for the *xyz*, *cif*, *dat*, *md*, and *cube* files are selected by "Examples" as shown below.
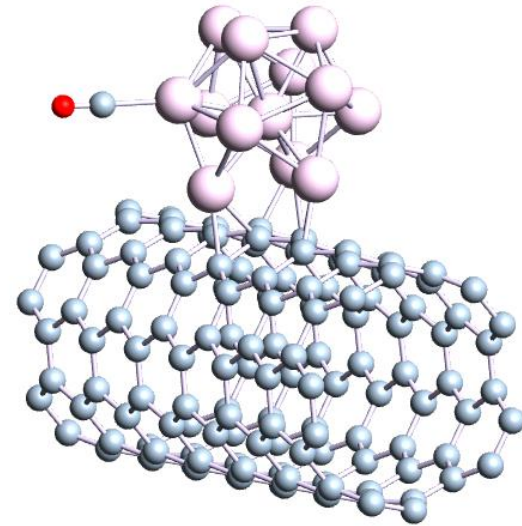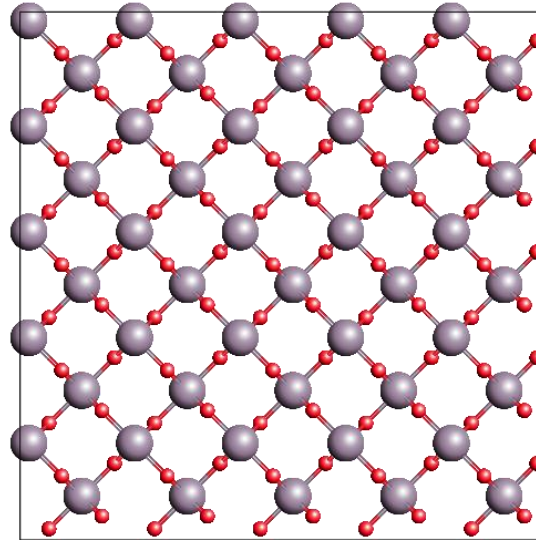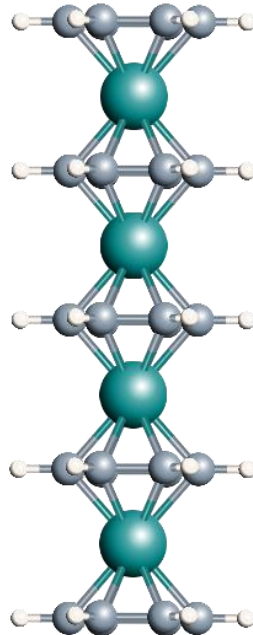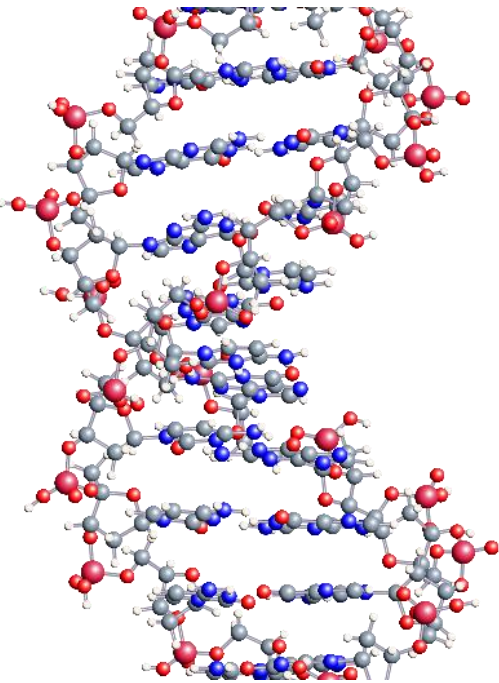
Atomic Attributes

Attributes of atoms can be changed by checking "Atomic Attributes". You will see the following a periodic table. By clicking one of elements, a small control panel pops up as shown below.
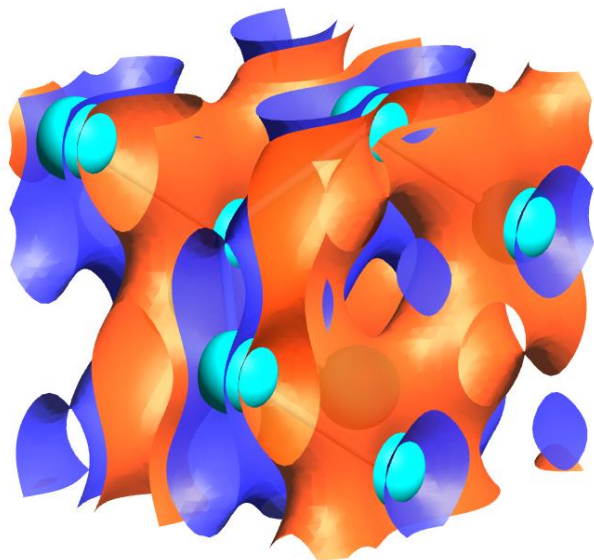
Visualization of cube files

- By dragging and dropping a cube file onto the web, one can visualize isosurfaces as shown below.

- On a control panel appearing the right top, one can select an algorithm such as marching cubes to calculate the isosurface, and control parameters such as isovalue, opacity, and color.
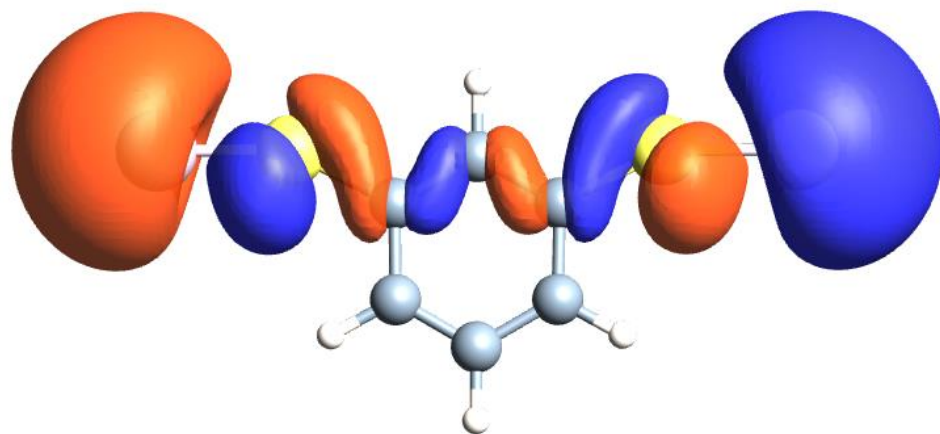
| Algorithm	Marching Cubes ⌄
Isovalue	0.016
Opacity	0.9
Facets	☑
Edges	☐
Positive_Isosurface	☑
Negative_Isosurface	☑
Color_Positive	0xf04410
Color_Negative	0x3333ff
Close Controls	

Visualization of the 1st Brillouin zone

Brillouin zone ☑ The 1ˢᵗ Brillouin zone is shown by checking "Brillouin zone",

and a suggested k-path is also depicted by the red lines for the band structure calculation. By clicking "Suggested k-path", you can download the k-path to a file. Also, the k-path will be included when you save an OpenMX input file. The generation of k-path is based on a paper: W. Setyawan and S. Curtarolo, Comp. Mat. Sci. 49, 299 (2010).

A common value is used to determine the Bravais lattice as tolerance of the length (Ang.) and angle (Deg.) of lattice vectors, which is controlled by "Tolerance".
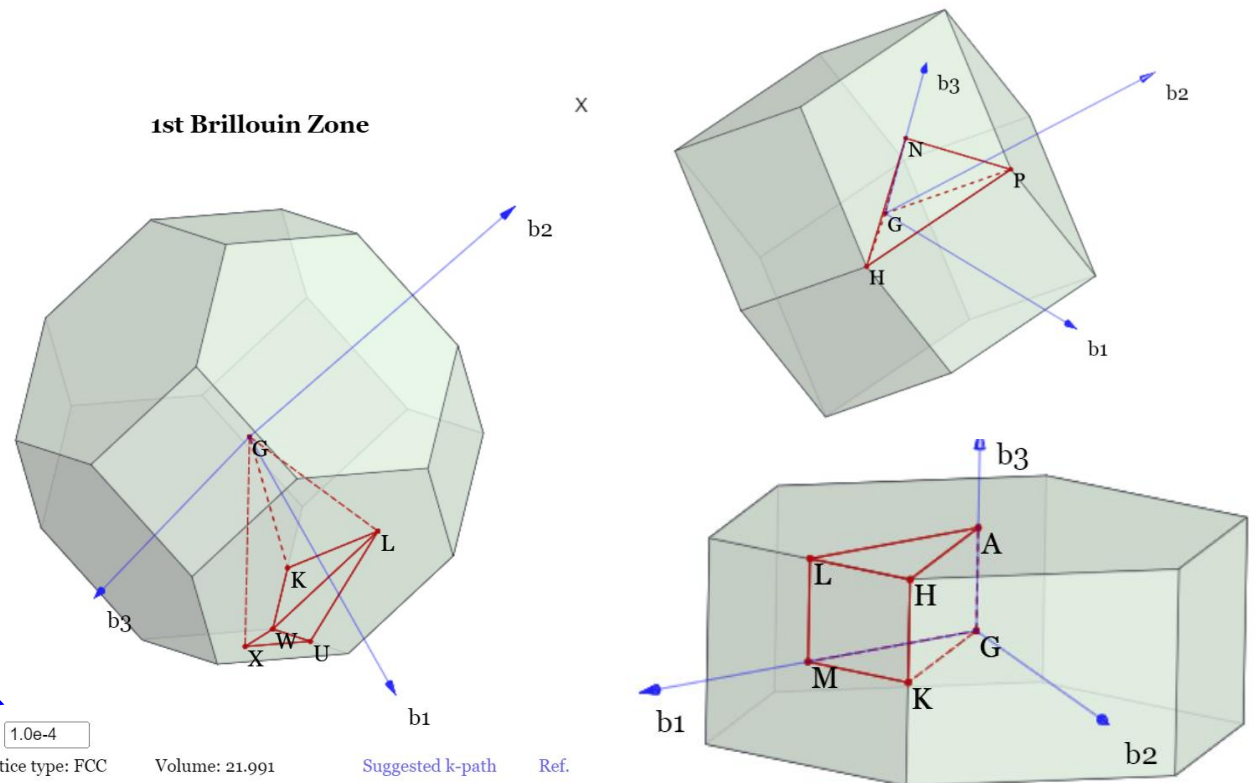

1st Brillouin Zone
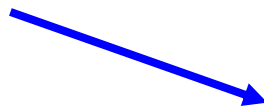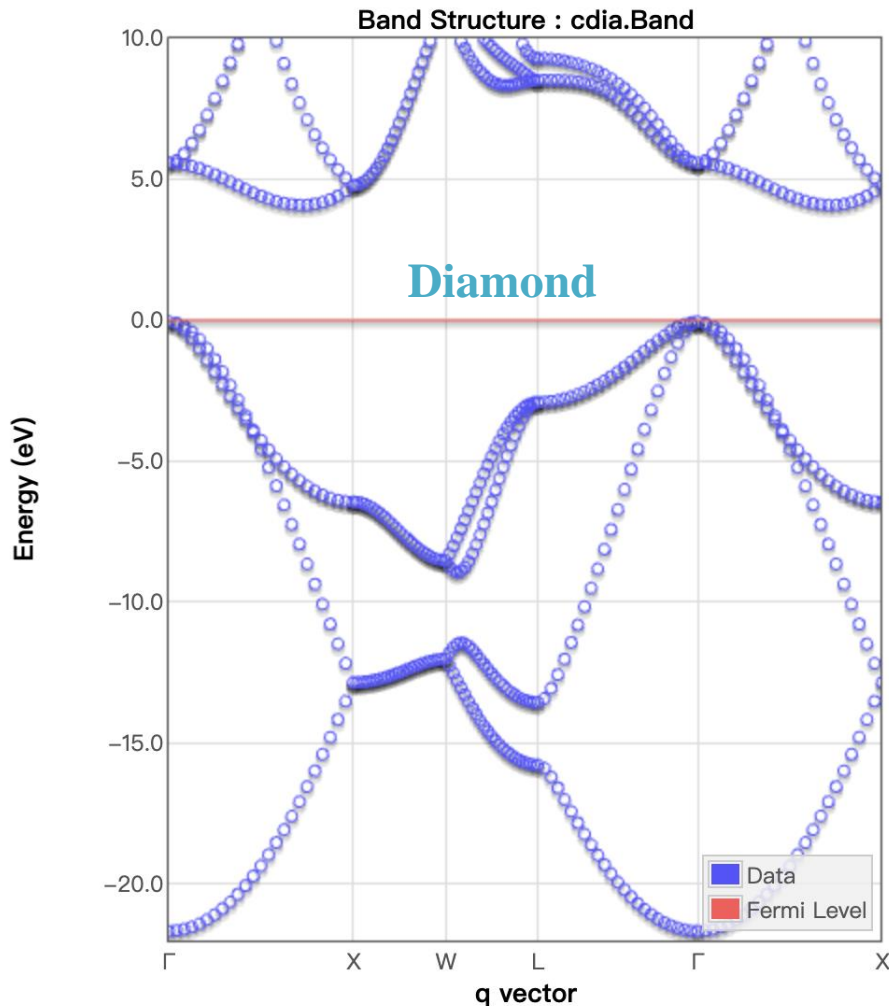
Tolerance 1.0e-4

Bravais lattice type: FCC   Volume: 21.991   Suggested k-path   Ref.

Band Structure Viewer

- By dragging and dropping a *.Band file onto the OpenMX Viewer webpage, one can visualize a band structure in a new tab.

Band Structure : cdia.Band

Diamond

- By pressing *mouse left button* and moving *cursor up/down*, the "Energy" range can be shifted.

- By scrolling *middle wheel button*, the "Energy" range can be scaled up/down.

- The Fermi-level line can be adjusted by controlling the "**Fermi_Level**" slider.

Energy_Unit	eV ⌄
Fermi_Level	-1.6
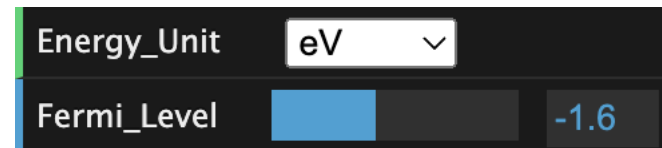
Prospects

- A simple structure builder has been being developed by Dr. Yung-Ting Lee, which enables us to manipulate the structure easily.

- The viewer functionality would be available as an API that could be called from the other web.

- The input file generator will be available on CUI via Node.js.

- Other visualizations of the volumetric 3D data such as isosurface plus scalar and vector information will be supported, e.g., local chemical potential analysis and Fermi surface.

- It would be possible to develop an integrated system that users can make structures, submit the corresponding job to machines a user resisters, and analyze the results.