Manual of 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.

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

The document provides the usage of the OpenMX Viewer.

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July 27, 2023

On license and citation of the related paper

- The OpenMX Viewer has been released under the practice of the GNU General Public License v3 (GPL).

  http://www.gnu.org/licenses/gpl-3.0.en.html

- We appreciate your citation of the following paper when you use the OpenMX Viewer for your research:

  "OpenMX Viewer: A web-based crystalline and molecular graphical user interface program",
  Y.-T. Lee and T. Ozaki, Journal of Molecular Graphics and Modelling 89, 192-198 (2019).

  https://doi.org/10.1016/j.jmgm.2019.03.013

Release notes

OpenMX Viewer:

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

Manual:

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

Web browsers we tested and recommended ones

So far, we have tested the OpenMX Viewer on the following browsers:

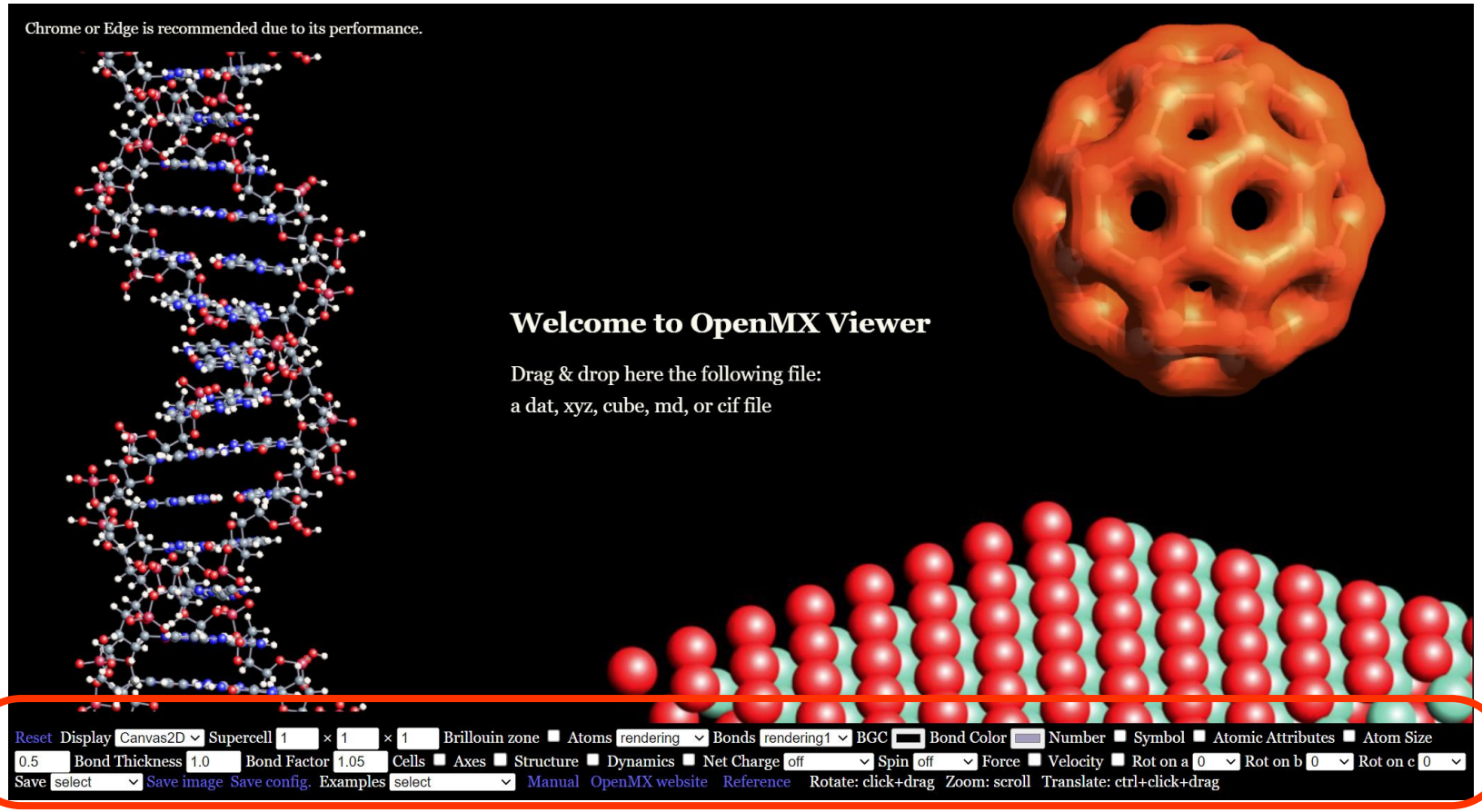
Chrome, Edge, Firefox, Opera, Safari, Waterfox, Brave, Vivaldi, SRWare, Avast, and Sleipnir.

Our test (Feb. 02, 2023) suggests that the OpenMX Viewer can be used without stress on Chrome and Edge due to its performance.

We would like to recommend you the use of these Web browsers.

Getting started with OpenMX Viewer

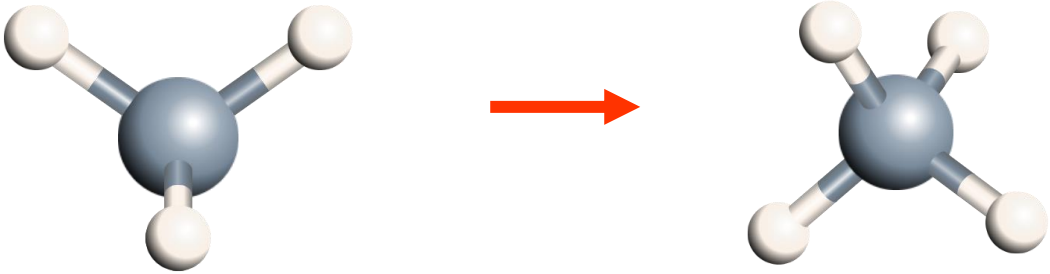
Visit the website: http://www.openmx-square.org/viewer/
and drag & drop a dat, xyz, cube, md, or cif file on the site.
Then, you will see the structure of your model.



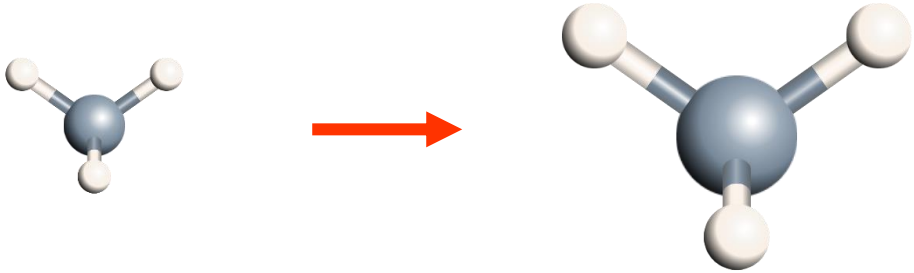
Here is the main control panel as we will explain in the next slides.

Rotation, zooming, and translation

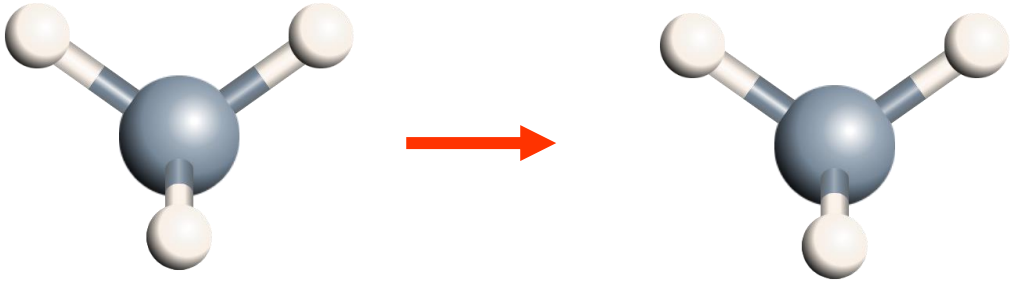
- You can rotate the structure by “click+drag”.



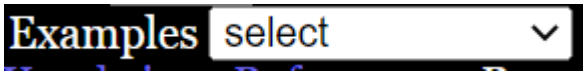
- You can zoom in and out the structure by “scroll”.



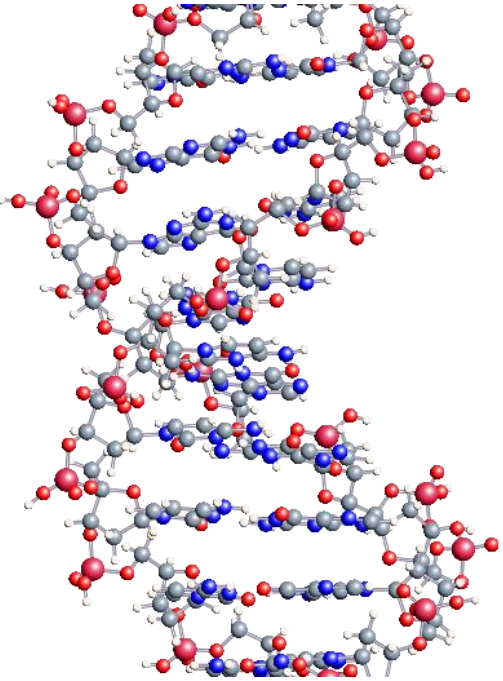
- You can translate the structure by “ctrl+click+drag”.

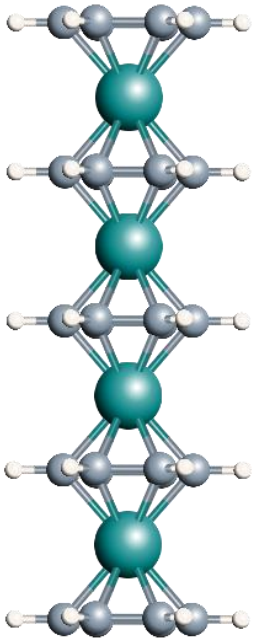


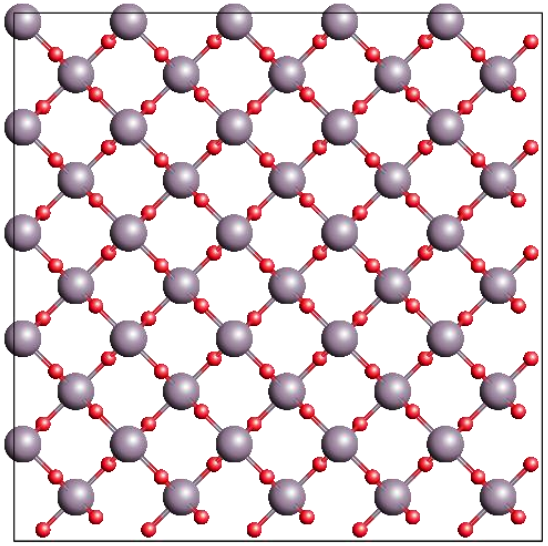
Examples

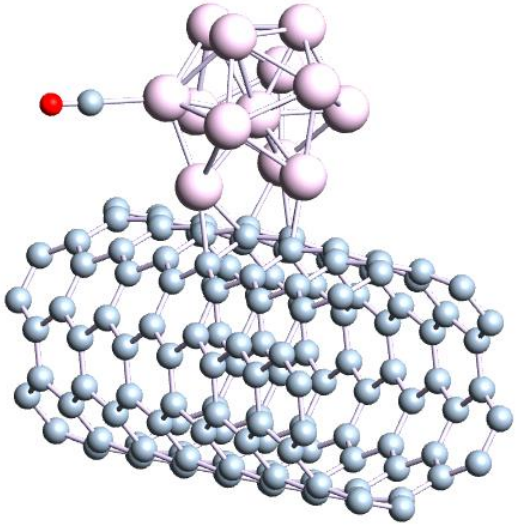


- Examples for the *xyz*, *cif*, *dat*, *md*, and *cube* files are selected by “Examples” as shown below.

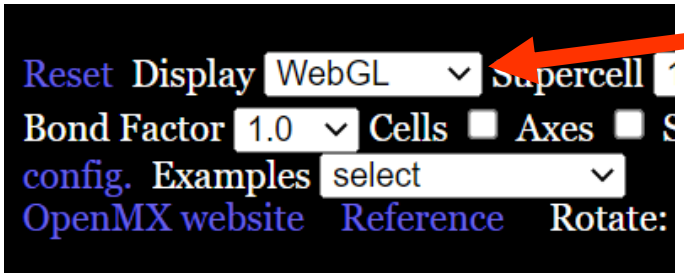






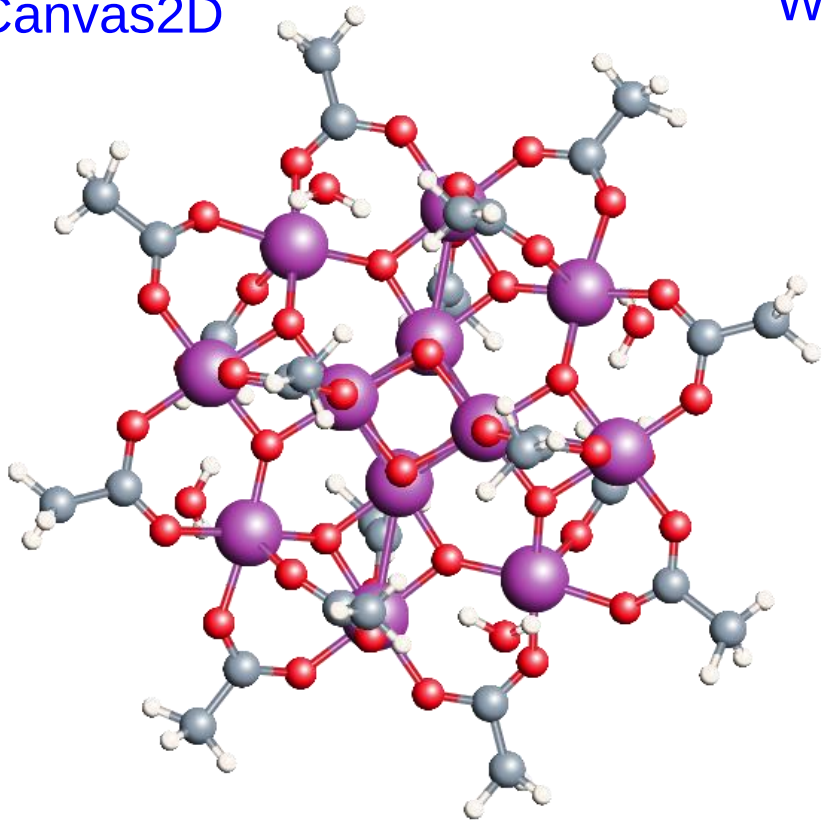


Canvas2D or WebGL

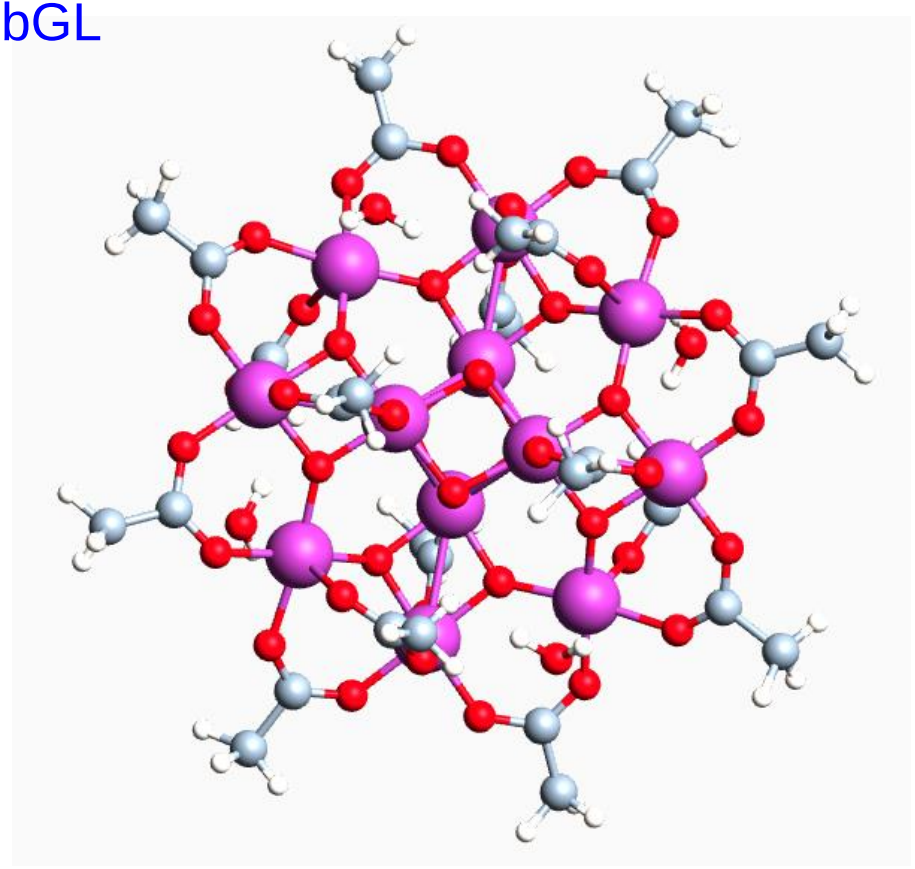


- The display style can be chosen as either Canvas2D or WebGL. The following is an example.

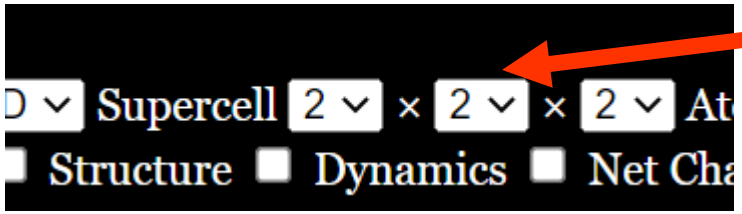
Canvas2D



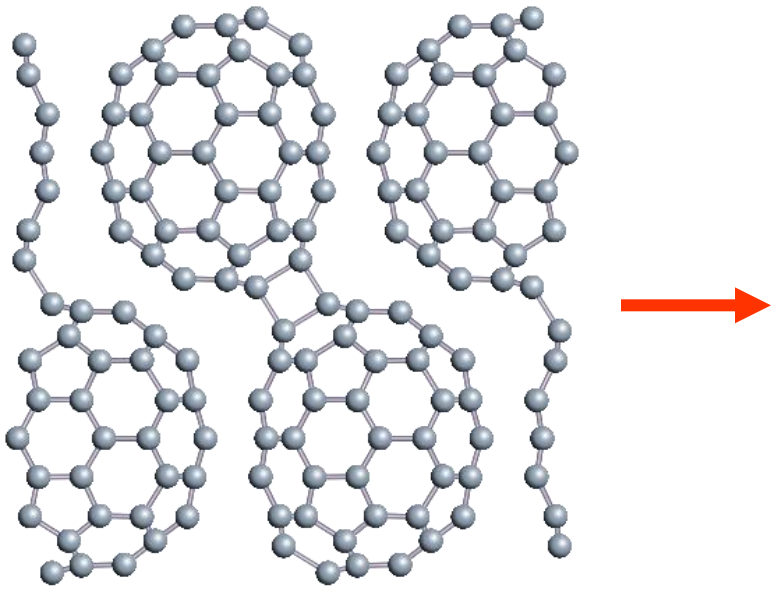
WebGL

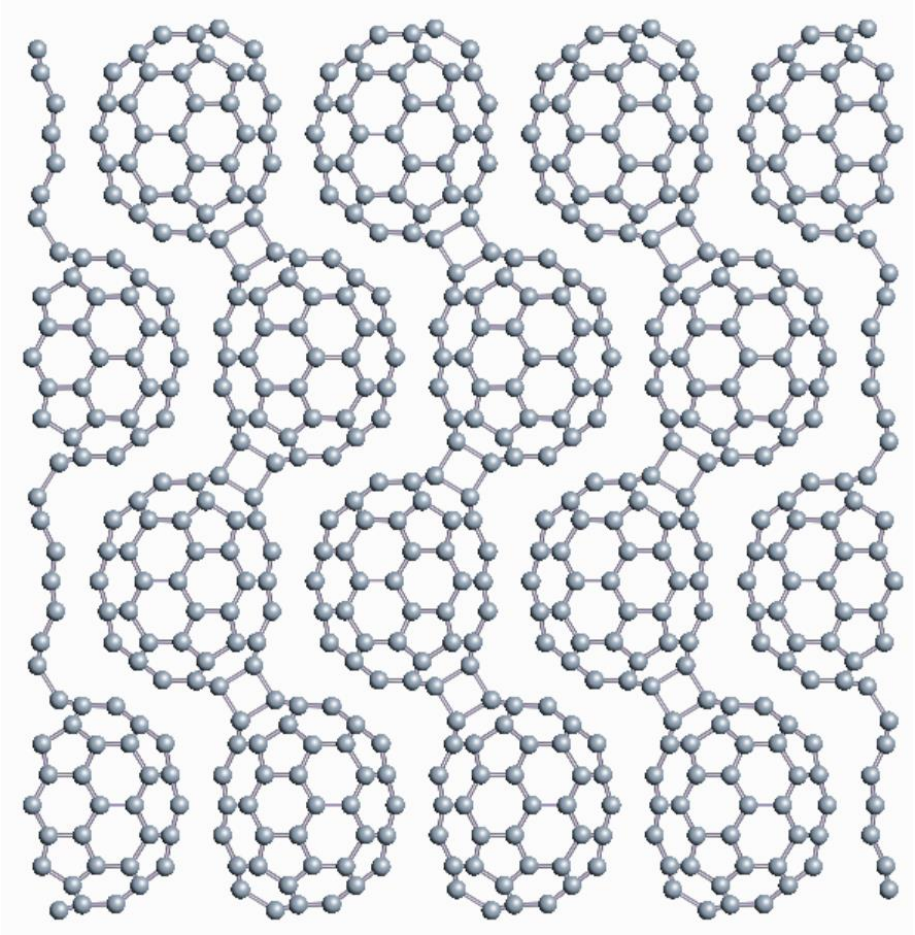


Supercell



- The supercell can be easily generated by selecting the number of cells along a-, b-, and c-axes.



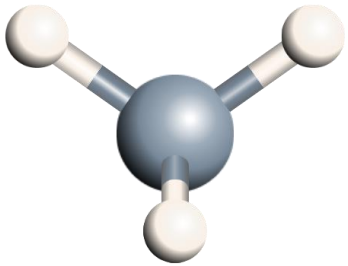


Display style of atoms and bonds

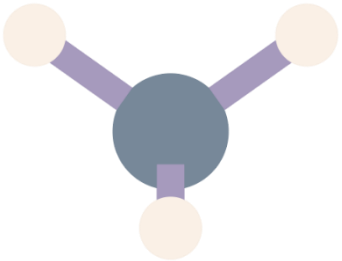
- The display styles of atoms and bonds are controlled by “Atoms” and “Bonds. The followings are examples.

- Canvas2D

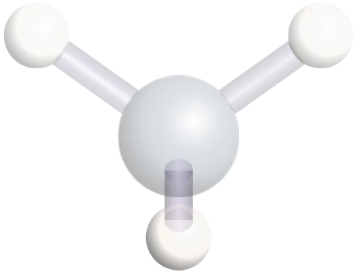
rendering1



solid+wire

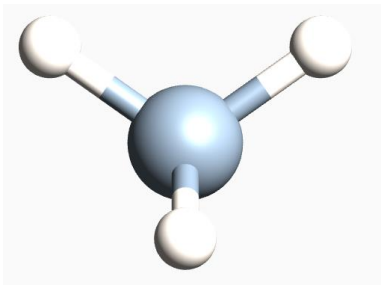


translucent

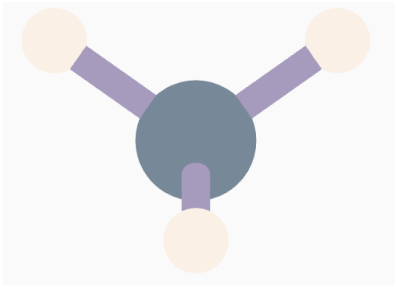


- WebGL

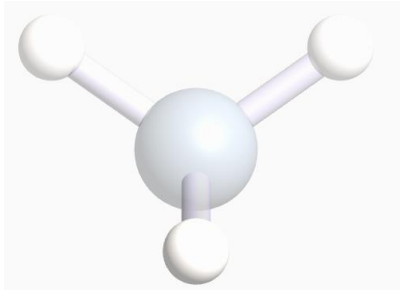
rendering1



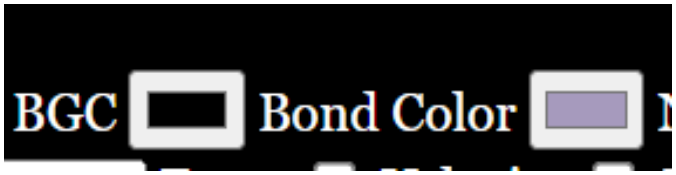
solid+wire

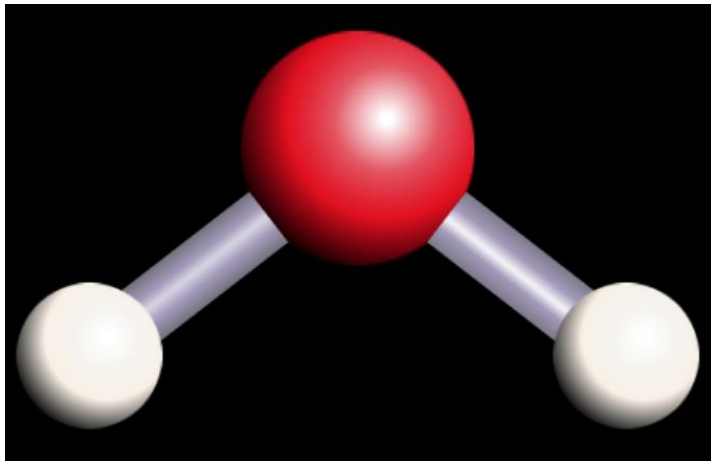


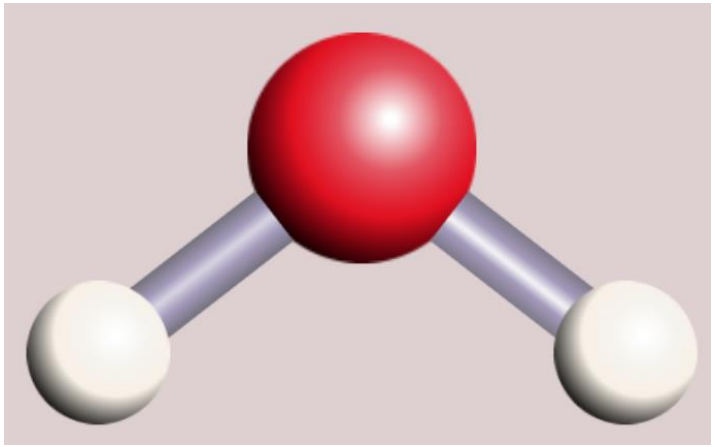
translucent



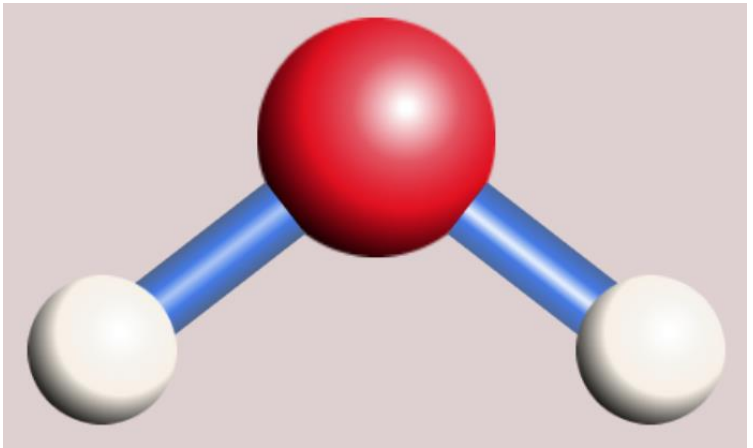
Background and bond colors







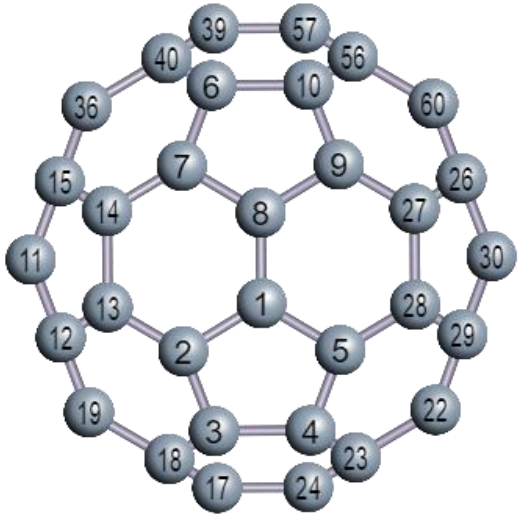
- The color of background can be changed by “BGC”, and the color of bonds can be controlled by “Bond Color” when “Bonds=rendering2” as shown below:



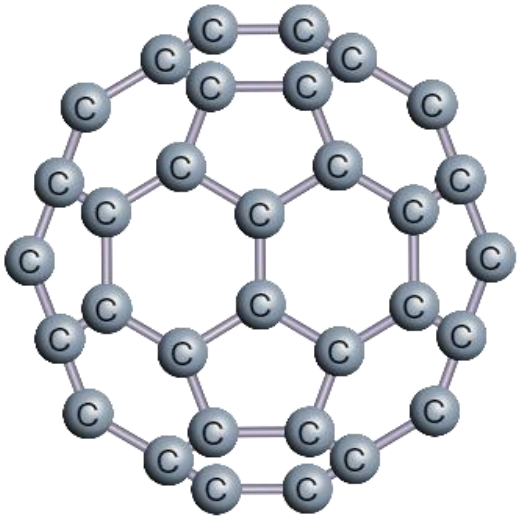
Displaying atomic serial number and symbol

- The serial number of atoms, atomic symbol, and both of them can be displayed by checking “Number” or/and “Symbol”.

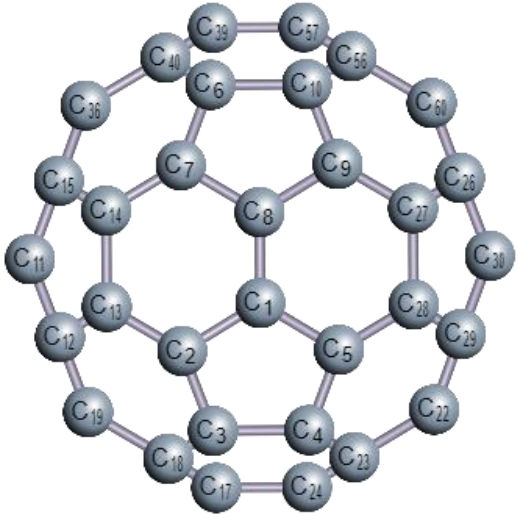
Number checked



Symbol checked

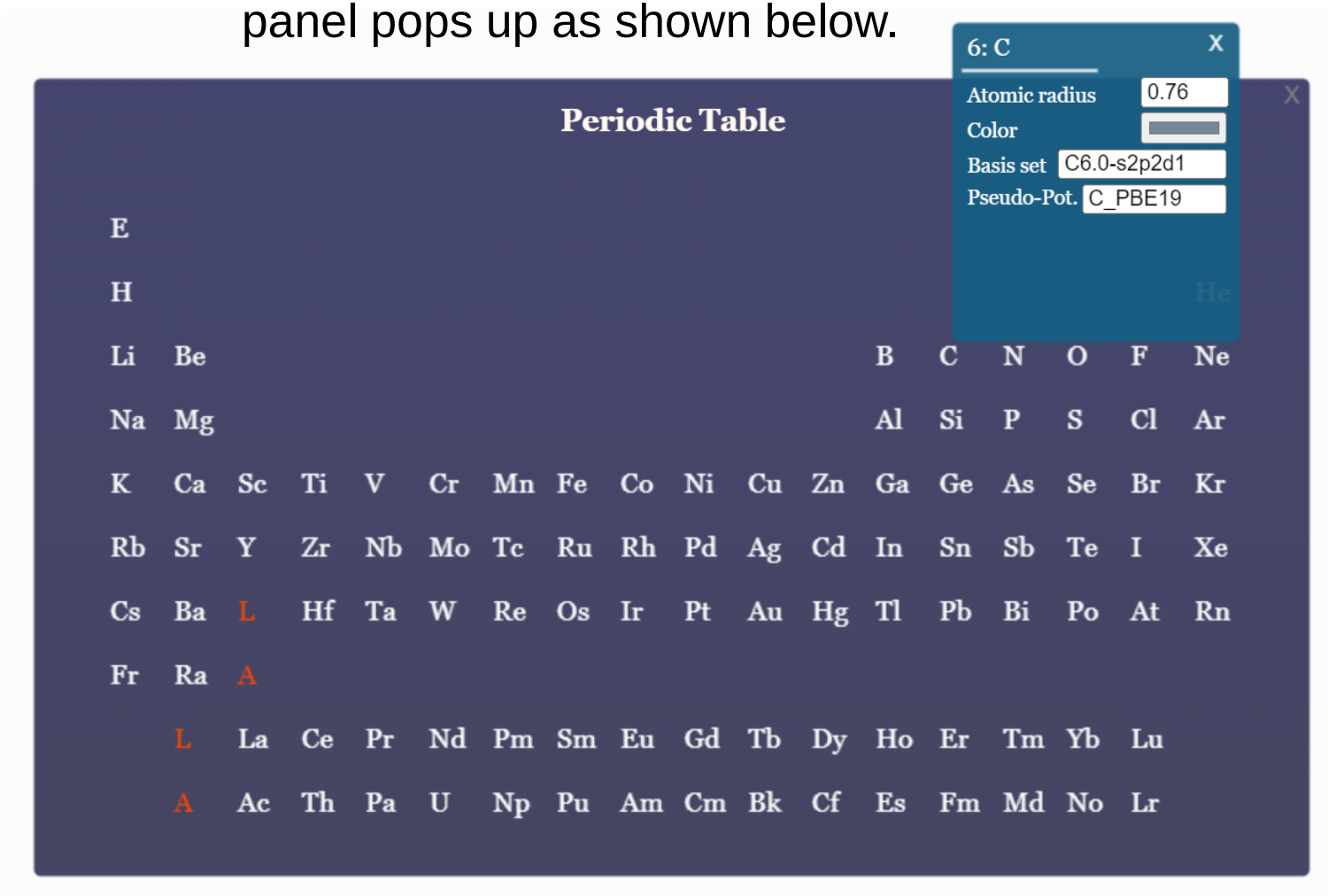


Number and *Symbol* checked



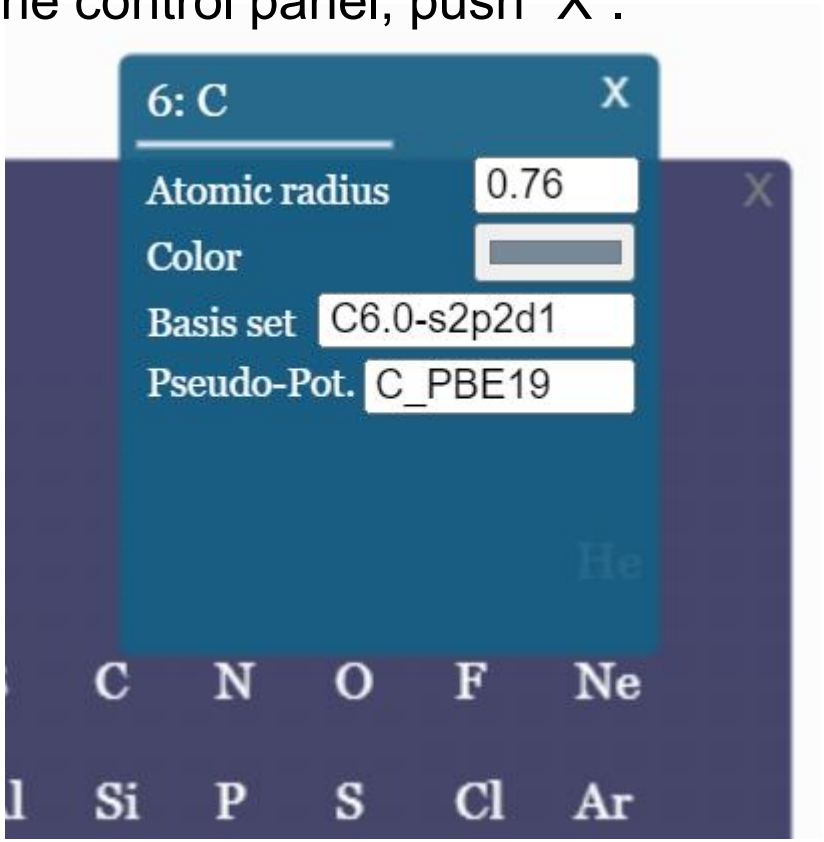
Atomic Attributes #1

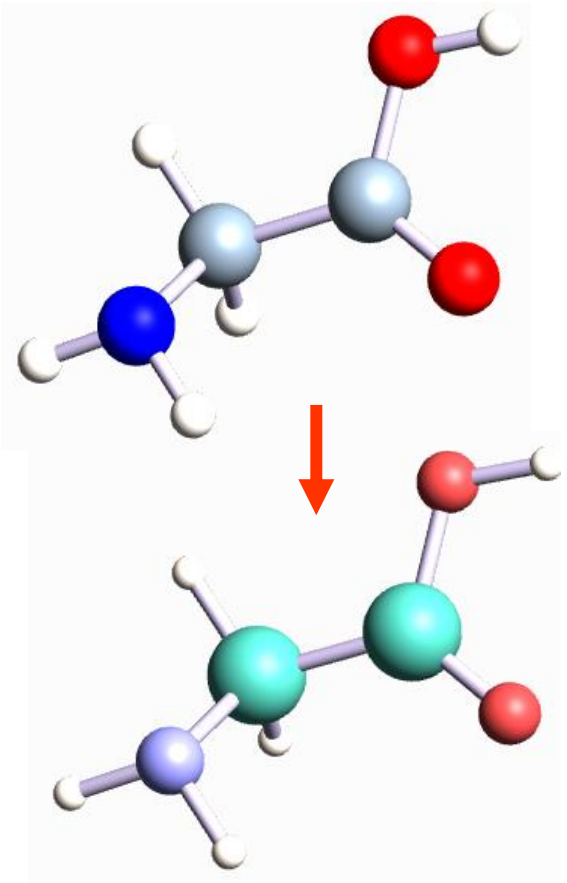
Attributes of atoms can be changed by checking “Atomic Attributes”. You will see the following a periodic table. By clicking one of elements, a small control panel pops up as shown below.



Atomic Attributes #2

- The radius, color, basis set, and peudopotential of each element can be changed in the control panel. By changing the radii and colors of elements, one can obtain a proper visualization depending on your sense. The following is an example. The setting of basis set and pseudopotential will be reflected in generating the input file. To close the control panel, push “X”.



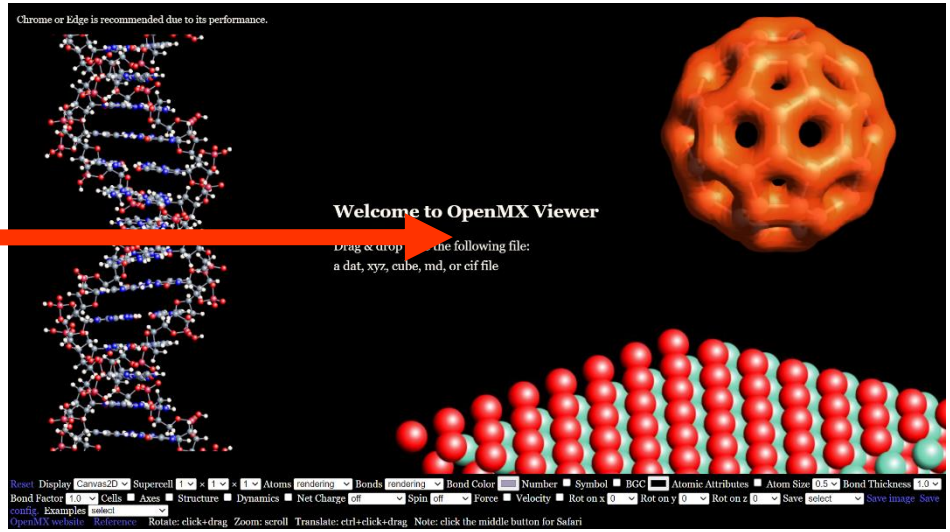


Atomic Attributes #3

- The settings by the control panel including the periodic table panel can be saved to a configuration file by clicking “Save config.”.

- In the next use, you can start with the configuration by dragging and dropping it onto the website of the OpenMX Viewer.

- Just drag&drop “omxv.config” onto the web to start with your configuration.

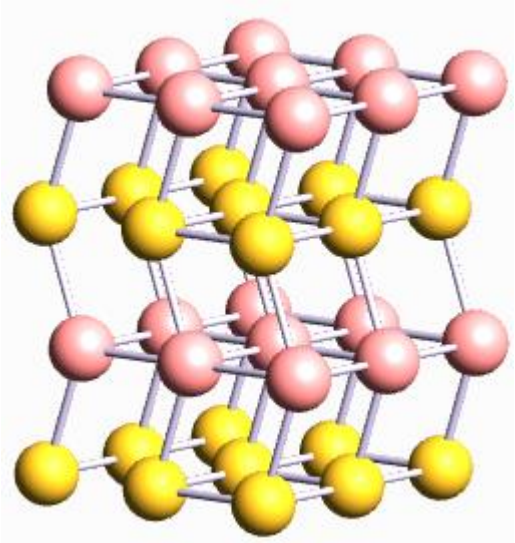


Atom Size and Bond Thickness

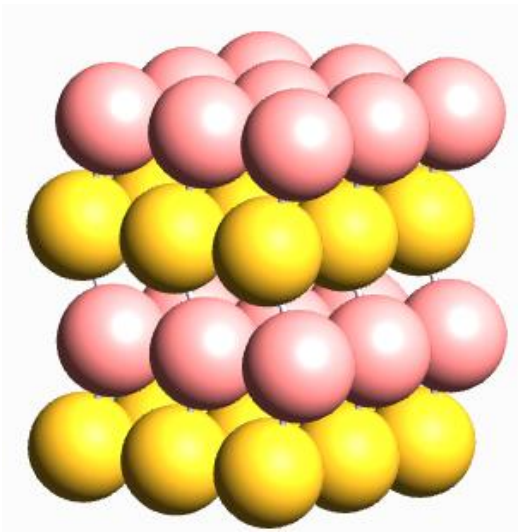
Atom Size 0.5 Bond Thickness 1.0

- The scaling factors for atomic radii and bond thickness are controlled by setting “Atom Size” and “Bond Thickness”, respectively, where the default values are set to 0.5 and 1.0, respectively. The following is an example.

Default



Atom Size = 1.0

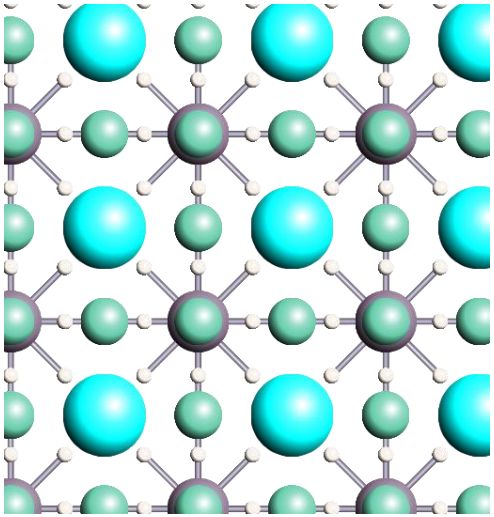


Bond Factor

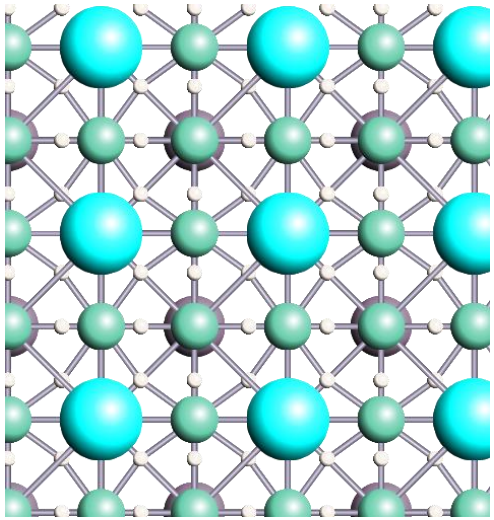
- As default, a bond is generated if the distance between two atoms is smaller than the sum of atomic radii.

- The threshold is changed by “Bond Factor” so that the bond can be formed if the distance between two atoms is smaller than the sum of atomic radii times the value of “Bond Factor”. Note that the default value is 1. The following is an example.

Default

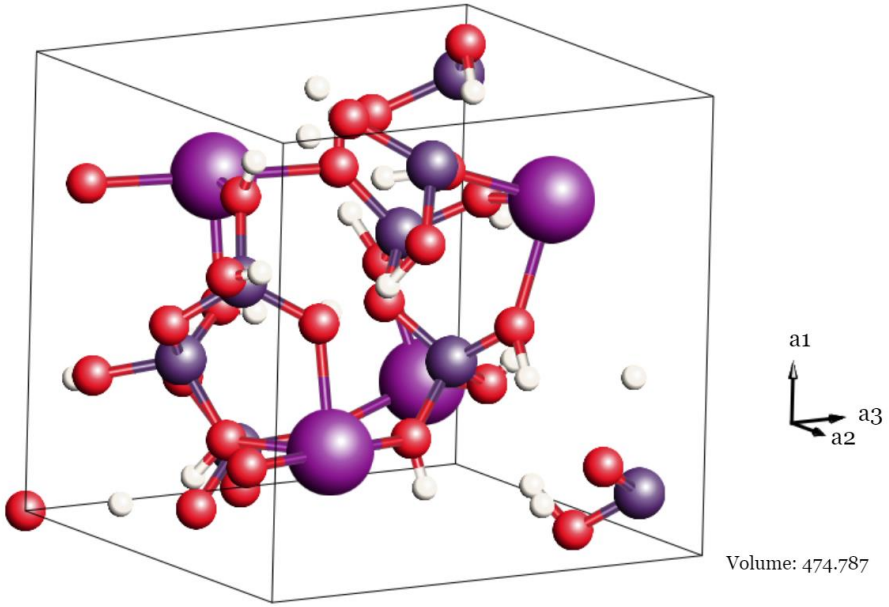


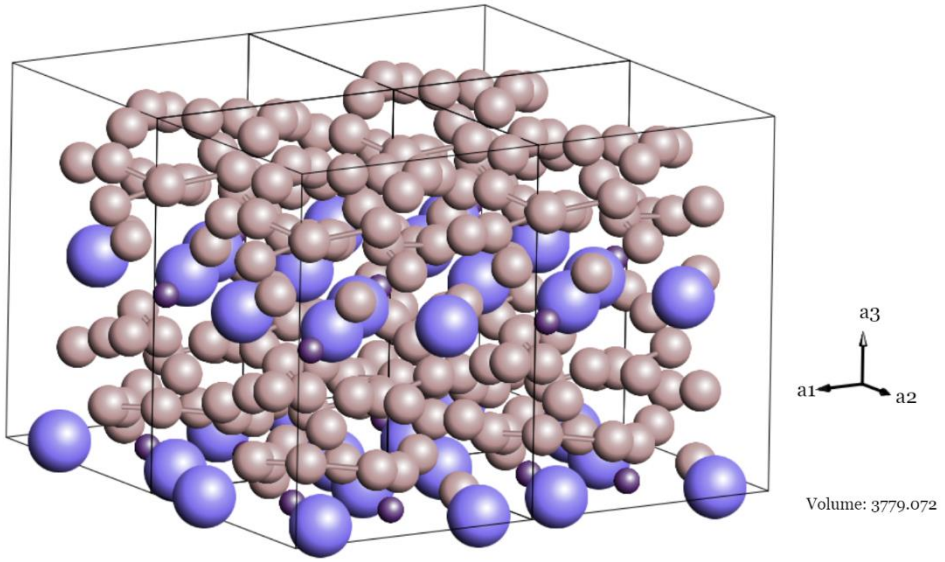
Bond Factor = 1.1



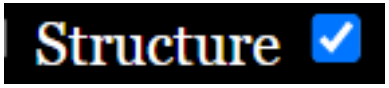
Cells and Axes

- The unit cells and axes are displayed by checking “Cells” and “Axes”, respectively. The followings are examples.





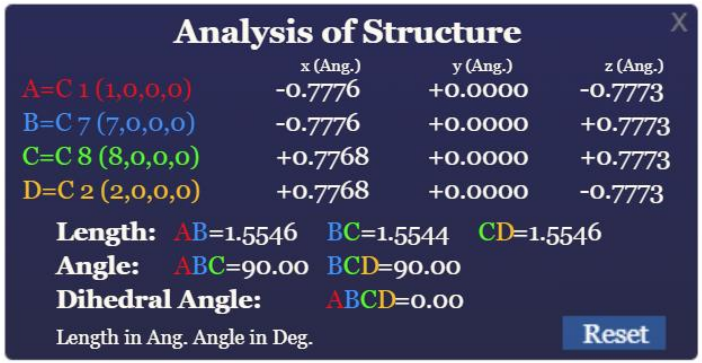
Analysis of Structure

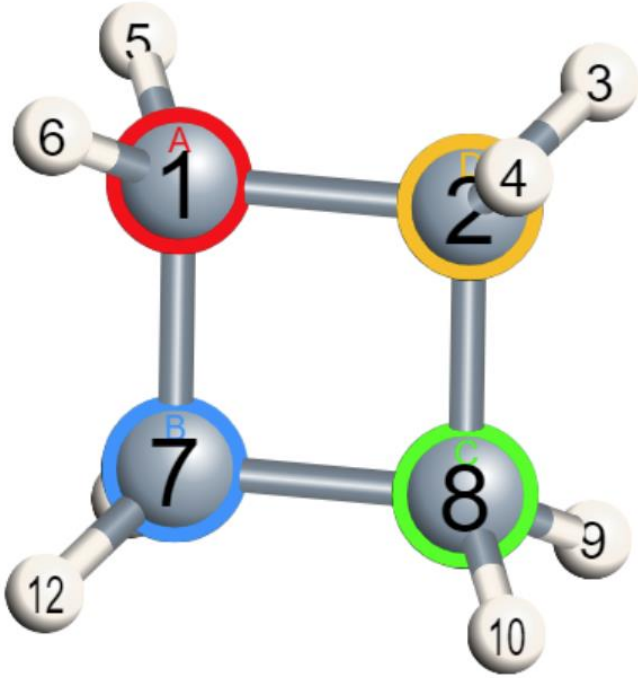


- The structure such as bond length and bond angle can be analyzed by clicking “Structure”. Then, a control panel pops up as shown below.

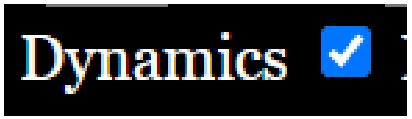
- Clicking atoms marks selected atoms with colored circles, and the bond length, angles, and dihedral angle are shown in the control panel. The position of the control panel can be moved by hanging “Analysis of Structure ”.

- To close the control panel, push “X”.

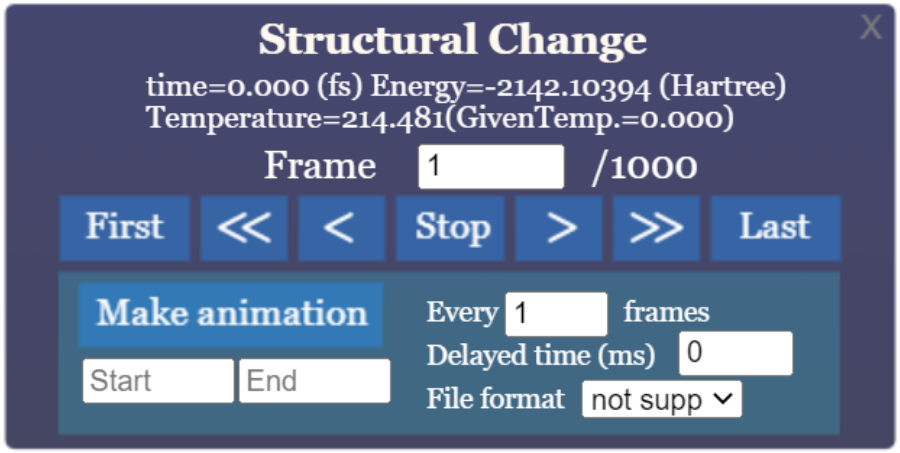




Animation for *xyz* and *md* files



- The xyz and md files can be animated by checking “Dynamics”. In this case, you will see a control panel as



- By pushing “<” and “>“, the frame of structures goes backward and forward, respectively.
- By “<<” and “>>”, the structure is animated towards backward and forward direction, respectively. Pushing “<<” and “>>” several times accelerates the display speed.
- The functionality of “Make animation” is not supported yet. So, please use a capture software to create video files. As for the format of md file, please see the next slide.

Format of the *md* file #1

- The *md* file, supported by OpenMX, is an extension of the *xyz* file, and the format is as follows:

1st step

```
10
time=    0.000 (fs) Energy= -56.61840 (Hartree) Temperature= 1000.000 (Given Temp.= 1000.000) Cell_Vectors= 10.18041  0.00000  0.00000  0.00000 10.18041  0.00000  0.00000  0.00000  8.55154
  C   -0.55502 -0.05167  0.35409   0.03654 -0.00779 -0.03763 -1394.21538 338.60117 -141.80824  -0.49099  0.00000  0.00000  0.00000
  C    0.81500 -0.46585 -0.13783  -0.18935 -0.00202  0.02830 992.13064 -1040.97544 103.16876   0.07147  0.00000  0.00000  0.00000
  O    0.86860 -1.67958 -0.73136  -0.14908 -0.15936 -0.04402 897.25381 825.75866 269.26108  -0.58253  0.00000  0.00000  0.00000
  N   -0.89697  1.28481 -0.17674  -0.00318 -0.04569 -0.07022 670.45601 -1105.81277 330.04574  -0.64593  0.00000  0.00000  0.00000
  H   -1.33580 -0.76012  0.00834  -0.03932 -0.04284 -0.01955 -3662.52988 -1946.83894 -2746.85085   0.20500  0.00000  0.00000  0.00000
  H   -0.54756 -0.10941  1.46450  -0.00875  0.00561  0.08037 3224.74855 -3639.73773 -1050.14409   0.15894  0.00000  0.00000  0.00000
  O    1.87095  0.13365 -0.04595   0.24840  0.16347  0.03671 -629.69966 -665.38792 848.63451  -0.57897  0.00000  0.00000  0.00000
  H    1.75863 -1.86736 -1.01311   0.11935 -0.01038 -0.03189 -3177.81107 145.86589 3824.88386   0.34050  0.00000  0.00000  0.00000
  H   -1.77844  1.56501  0.19676  -0.09529  0.03530  0.03816 2071.02647 -3750.21792 2529.07325   0.24358  0.00000  0.00000  0.00000
  H   -0.19940  1.95052  0.08130   0.07811  0.06151  0.02131 255.20767 -67.42941 4967.87871   0.27892  0.00000  0.00000  0.00000
```

2nd step

```
10
time=    0.200 (fs) Energy= -56.61485 (Hartree) Temperature= 1000.000 (Given Temp.= 1000.000) Cell_Vectors= 10.18041  0.00000  0.00000  0.00000 10.18041  0.00000  0.00000  0.00000  8.55154
  C   -0.55777 -0.05100  0.35377   0.03487 -0.01511 -0.04015 -1394.21538 338.60117 -141.80824  -0.48748  0.00000  0.00000  0.00000
  C    0.81683 -0.46794 -0.13760  -0.19595 -0.00079  0.02998 992.13064 -1040.97544 103.16876   0.07137  0.00000  0.00000  0.00000
  O    0.87030 -1.67803 -0.73085  -0.15944 -0.15994 -0.04333 897.25381 825.75866 269.26108  -0.58701  0.00000  0.00000  0.00000
  N   -0.89564  1.28257 -0.17613   0.00130 -0.04063 -0.07086 670.45601 -1105.81277 330.04574  -0.64508  0.00000  0.00000  0.00000
  H   -1.34350 -0.76443  0.00265  -0.03445 -0.03836 -0.01723 -3662.52988 -1946.83894 -2746.85085   0.20217  0.00000  0.00000  0.00000
  H   -0.54120 -0.11663  1.46319  -0.00903  0.00540  0.08059 3224.74855 -3639.73773 -1050.14409   0.15931  0.00000  0.00000  0.00000
  O    1.86985  0.13242 -0.04423   0.25269  0.16668  0.03755 -629.69966 -665.38792 848.63451  -0.58053  0.00000  0.00000  0.00000
  H    1.75346 -1.86717 -1.00578   0.13010 -0.01354 -0.03481 -3177.81107 145.86589 3824.88386   0.34479  0.00000  0.00000  0.00000
  H   -1.77523  1.55786  0.20219  -0.09718  0.03597  0.03909 2071.02647 -3750.21792 2529.07325   0.24466  0.00000  0.00000  0.00000
  H   -0.19812  1.95100  0.09144   0.07457  0.05823  0.02067 255.20767 -67.42941 4967.87871   0.27779  0.00000  0.00000  0.00000
10
time=    0.400 (fs) Energy= -56.61317 (Hartree) Temperature= 1000.000 (Given Temp.= 1000.000) Cell_Vectors= 10.18041  0.00000  0.00000  0.00000 10.18041  0.00000  0.00000  0.00000  8.55154
  C   -0.56059 -0.05034  0.35337   0.03267 -0.02305 -0.04150 -1422.28190 339.93279 -182.46142  -0.48282  0.00000  0.00000  0.00000
  C    0.81840 -0.47011 -0.13730  -0.20117  0.00108  0.03168 865.04417 -1085.02515 133.18142   0.07108  0.00000  0.00000  0.00000
  O    0.87187 -1.67661 -0.73037  -0.16673 -0.16130 -0.04381 831.90187 757.06130 252.42603  -0.59010  0.00000  0.00000  0.00000
.....
```

- Each block of data corresponds to each structural step as shown above, and the format of each block will be explained in the next slide.

Format of the *md* file #2

- Each block of the *md* file has the following format:

```
 10
time=    0.000 (fs) Energy= -56.61840 (Hartree) Temperature= 1000.000 (Given Temp.= 1000.000) Cell_Vectors= 10.18041  0.00000  0.00000  0.00000 10.18041  0.00000  0.00000  0.00000  8.55154
   C   -0.55502 -0.05167  0.35409   0.03654 -0.00779 -0.03763 -1394.21538 338.60117 -141.80824  -0.49099  0.00000  0.00000  0.00000
   C    0.81500 -0.46585 -0.13783  -0.18935 -0.00202  0.02830 992.13064 -1040.97544 103.16876   0.07147  0.00000  0.00000  0.00000
   O    0.86860 -1.67958 -0.73136  -0.14908 -0.15936 -0.04402 897.25381 825.75866 269.26108  -0.58253  0.00000  0.00000  0.00000
   N   -0.89697  1.28481 -0.17674  -0.00318 -0.04569 -0.07022 670.45601 -1105.81277 330.04574  -0.64593  0.00000  0.00000  0.00000
   H   -1.33580 -0.76012  0.00834  -0.03932 -0.04284 -0.01955 -3662.52988 -1946.83894 -2746.85085   0.20500  0.00000  0.00000  0.00000
   H   -0.54756 -0.10941  1.46450  -0.00875  0.00561  0.08037 3224.74855 -3639.73773 -1050.14409   0.15894  0.00000  0.00000  0.00000
   O    1.87095  0.13365 -0.04595   0.24840  0.16347  0.03671 -629.69966 -665.38792 848.63451  -0.57897  0.00000  0.00000  0.00000
   H    1.75863 -1.86736 -1.01311   0.11935 -0.01038 -0.03189 -3177.81107 145.86589 3824.88386   0.34050  0.00000  0.00000  0.00000
   H   -1.77844  1.56501  0.19676  -0.09529  0.03530  0.03816 2071.02647 -3750.21792 2529.07325   0.24358  0.00000  0.00000  0.00000
   H   -0.19940  1.95052  0.08130   0.07811  0.06151  0.02131 255.20767 -67.42941 4967.87871   0.27892  0.00000  0.00000  0.00000
```

- Each line in each block corresponds to the following information:

1st line: the number of atoms

2nd line: The text before "Cell_Vectors=.." is a comment. The "Cell_Vectors=" is a keyword to provide cell vectors, **a**, **b**, **c**. They are arranged as a_x, a_y, a_z, b_x, b_y, b_z, c_x, c_y, and c_z in Angstrom unit.

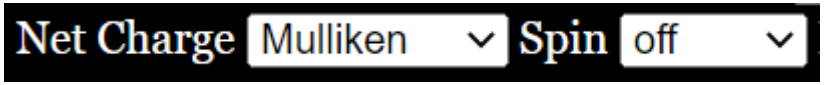
3rd to the last lines:

atomic symbol, x-, y-, z-coordinates in Angstrom unit, x-, y-, z-components of force in Hartree/Bohr, x-, y-, z-components of velocity in m/sec., net charge (electron charge is defined to be negative), local magnetic moment in Bohr magneton, Euler angles of spin in degree.

- An animated *xyz* file has a similar format, but the *md* file includes the information of cell vectors explicitly.

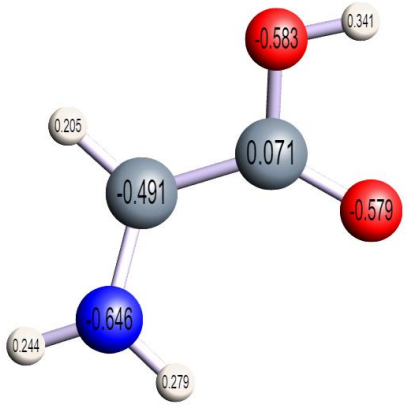
Net charge and Spin

- The information of net charge and spin stored in a md file can be analyzed by “Net Charge” and “Spin”, respectively.



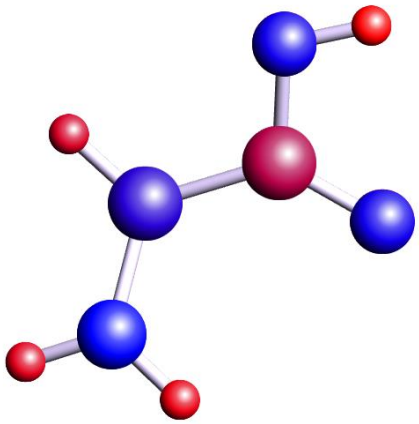
- The followings are examples.

Net Charge = Mulliken



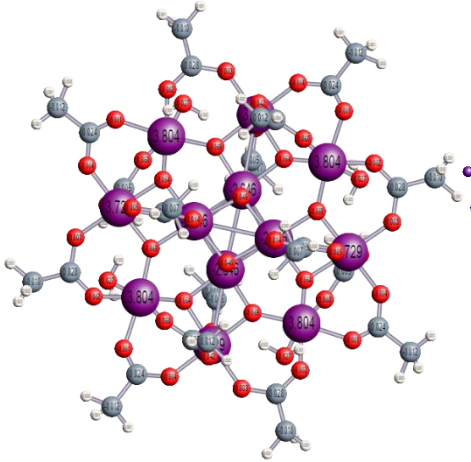
The net charge calculated by Mulliken population is shown on each atom, where zero means the neutral.

Net Charge = Mulliken-C



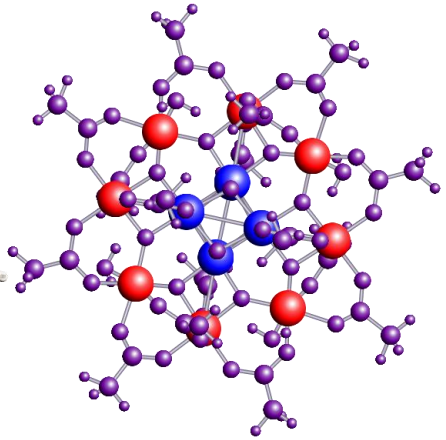
The net charge calculated by Mulliken population is shown by color, where the red and blue colors correspond to positive and negative, respectively.

Spin = spin



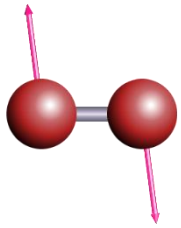
The local spin moment of each atom is shown in Bohr magneton.

Spin = spin-C



The local spin moment of each atom is shown by color, where the red and blue colors correspond to up- and down spin states, respectively.

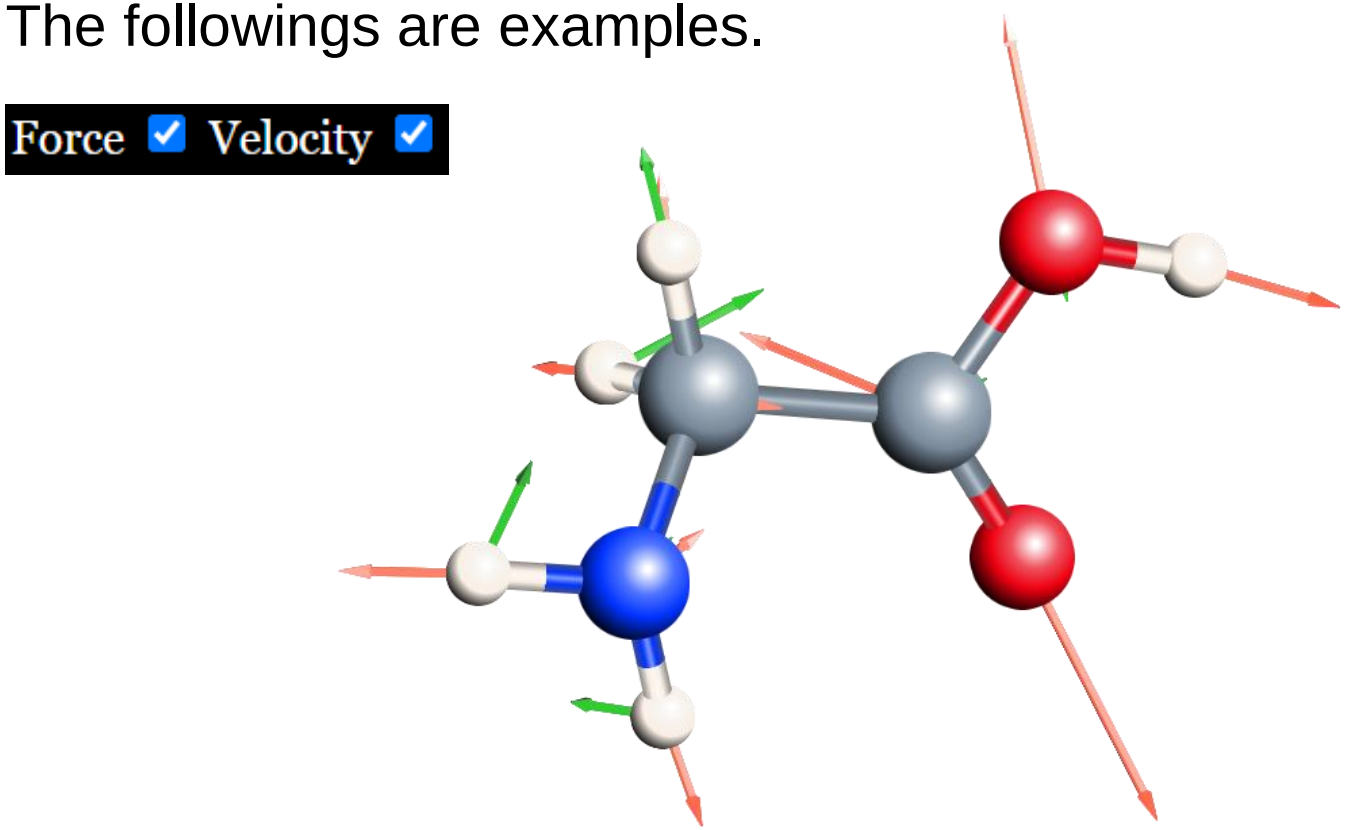
Spin = spin-V



The non-collinear local spin moment of each atom is shown by a vector style.

Force and Velocity

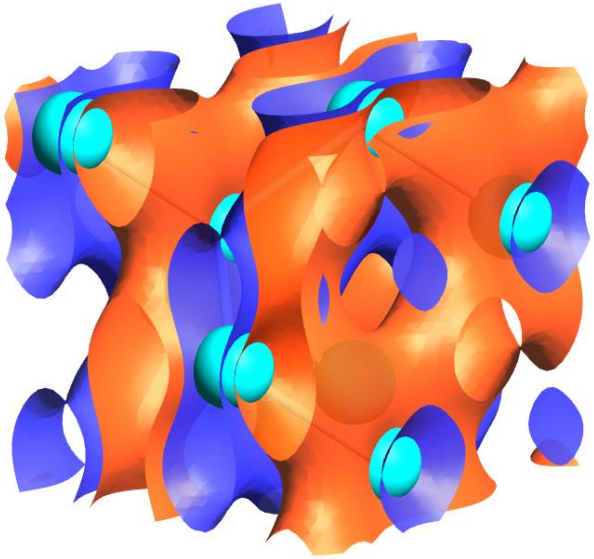
- The information of force and velocity stored in a md file can be analyzed by checking “Force” and “Velocity”, respectively. The followings are examples.

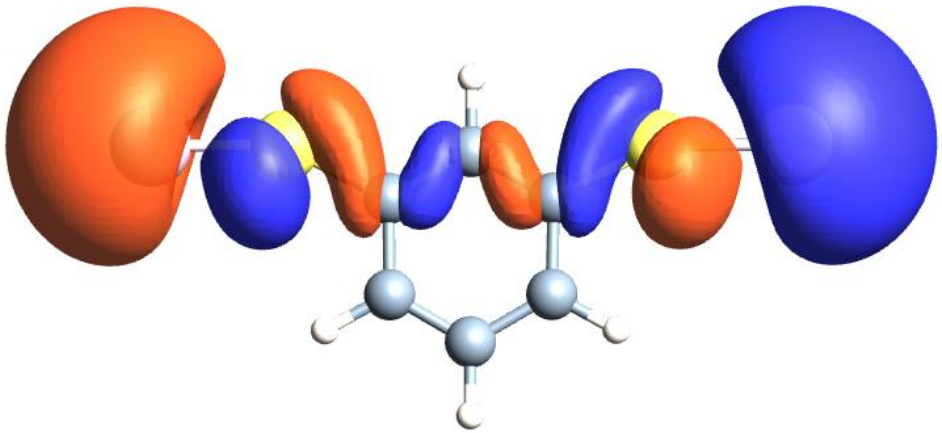


- The red and green arrows correspond to the force and velocity, respectively.

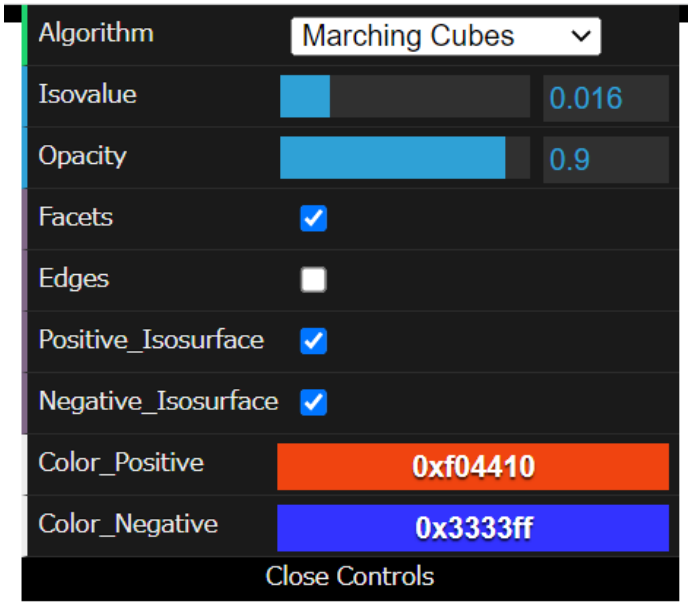
Visualization of cube files

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





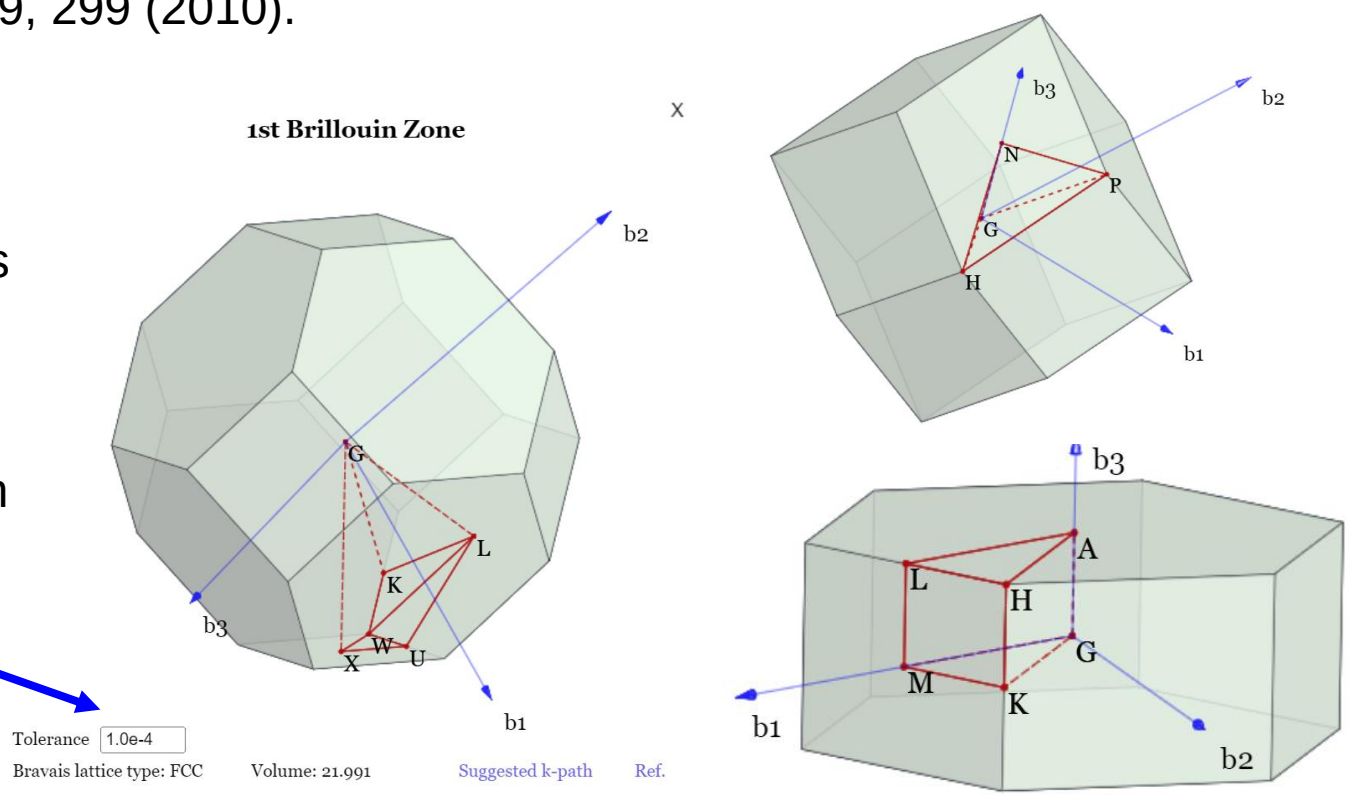
- On a control panel appearing the right top, one can select an algorithm such as marching cubes to calculate the isosurface, and control parameters such as isovalue, opacity, and color.



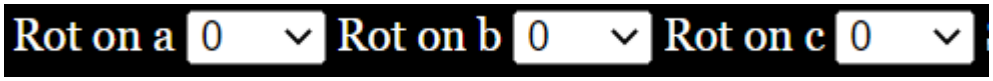
Visualization of 1st Brillouin zone

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”.

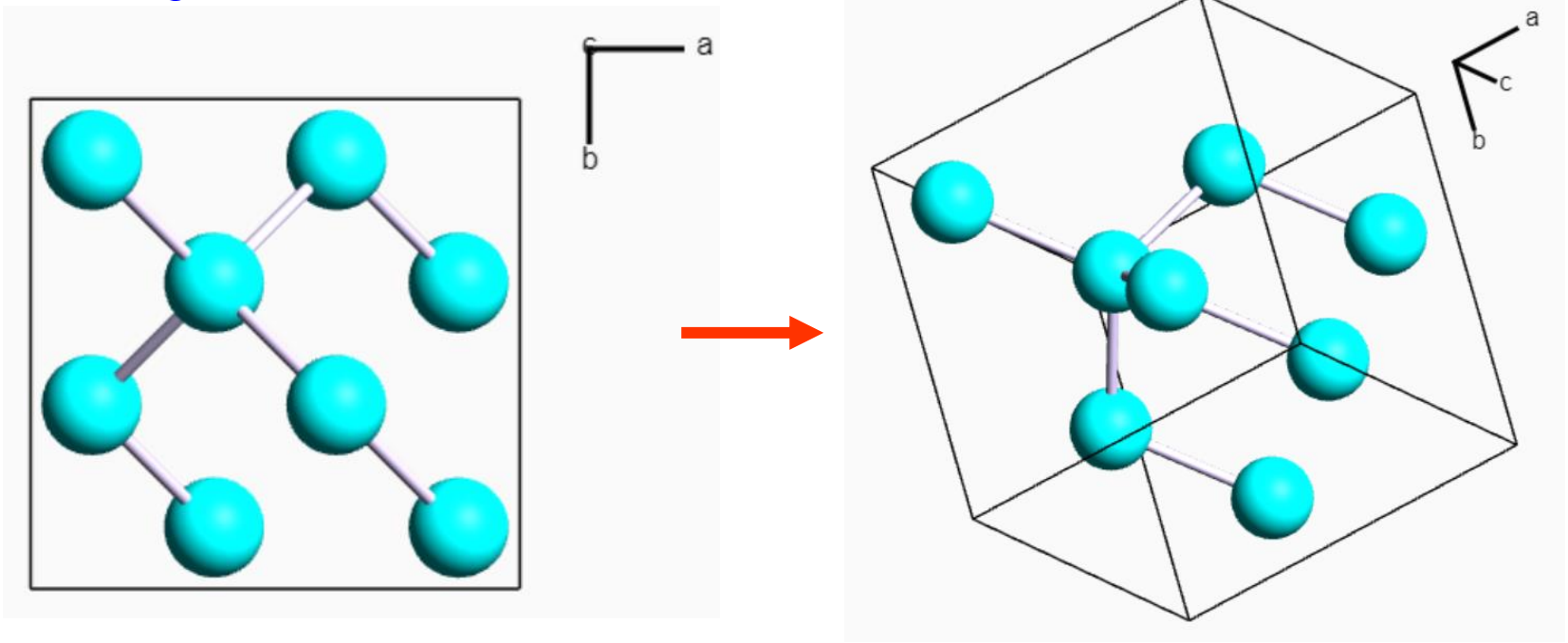


Rot on a-, b-, or c-axis

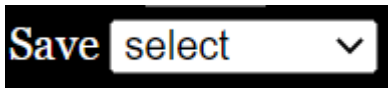


- The specific rotations of the structure can be performed by “Rot on a”, “Rot on b”, or “Rot on c” for on a-, b-, or c-axis, respectively. The following is an example.

Rotation on b-axis with 30 degree and then rotation on a-axis with 30 degree



Saving xyz, cif, and OpenMX input files



- You can save the structure as a *xyz*, *cif*, or OpenMX input files (*dat* file) by “Save”.

- By selecting one of the formats, a file is automatically saved as abc.(*xyz*, *cif,* or *dat*). The *dat* file can be saved with either xyz or fractional coordinates, and setting the basis sets and pseudopotential can be done through “Atomic Attributes”.

- The *dat* files can be used as the input files for OpenMX calculations.

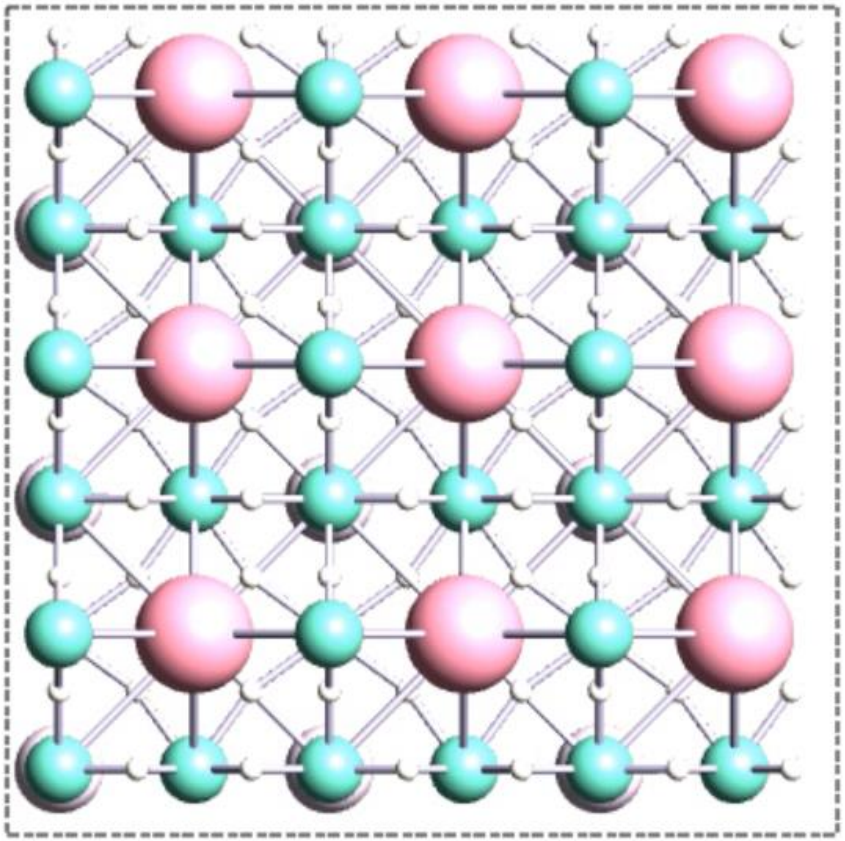
- Also, note that the input file for a supercell can be easily generated.

Saving image

- The structure can be captured as image by pushing “Save image”, and saved as a png file.

Save image

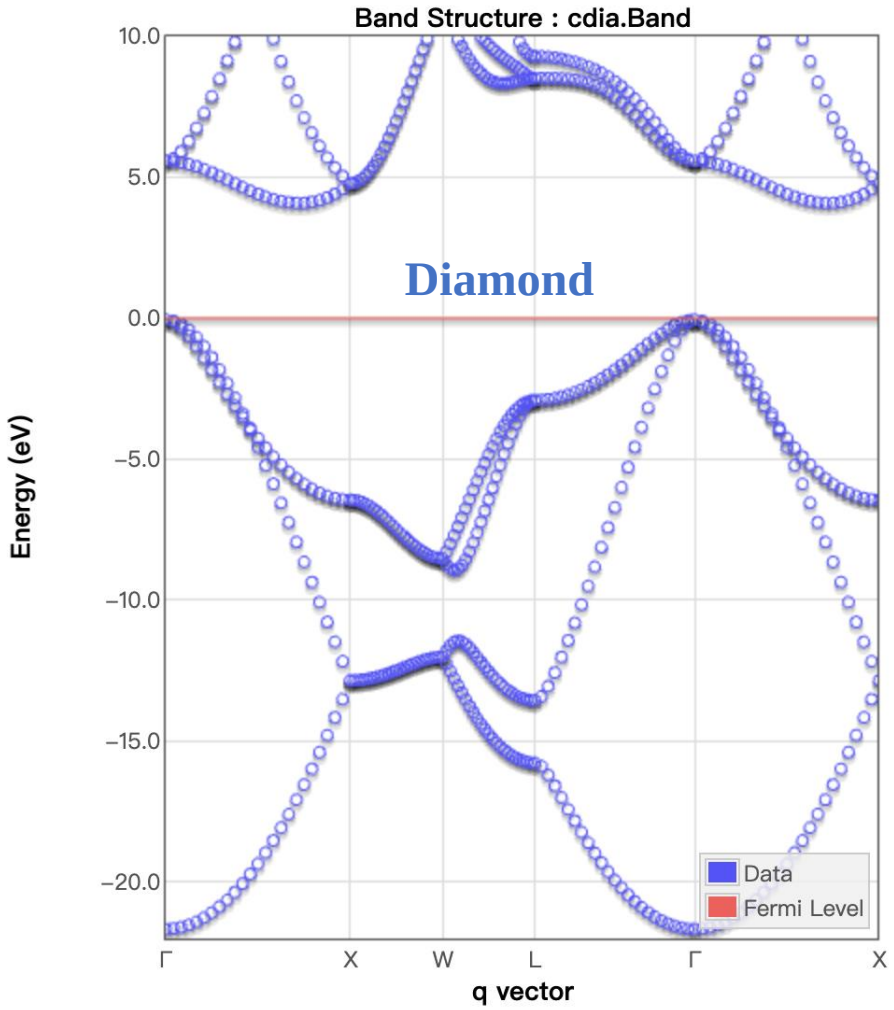
- After pushing “Save image”, and you can select a rectangular region to be saved using mouse as shown below.



- After selecting the rectangular region, the region is automatically saved as a png file of which quality can be better than that by another capture tool.

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.



- 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.

Bug report and request for development

- Any bug reports and request for development should be posted on the OpenMX Forum:

http://www.openmx-square.org/forum/patio.cgi